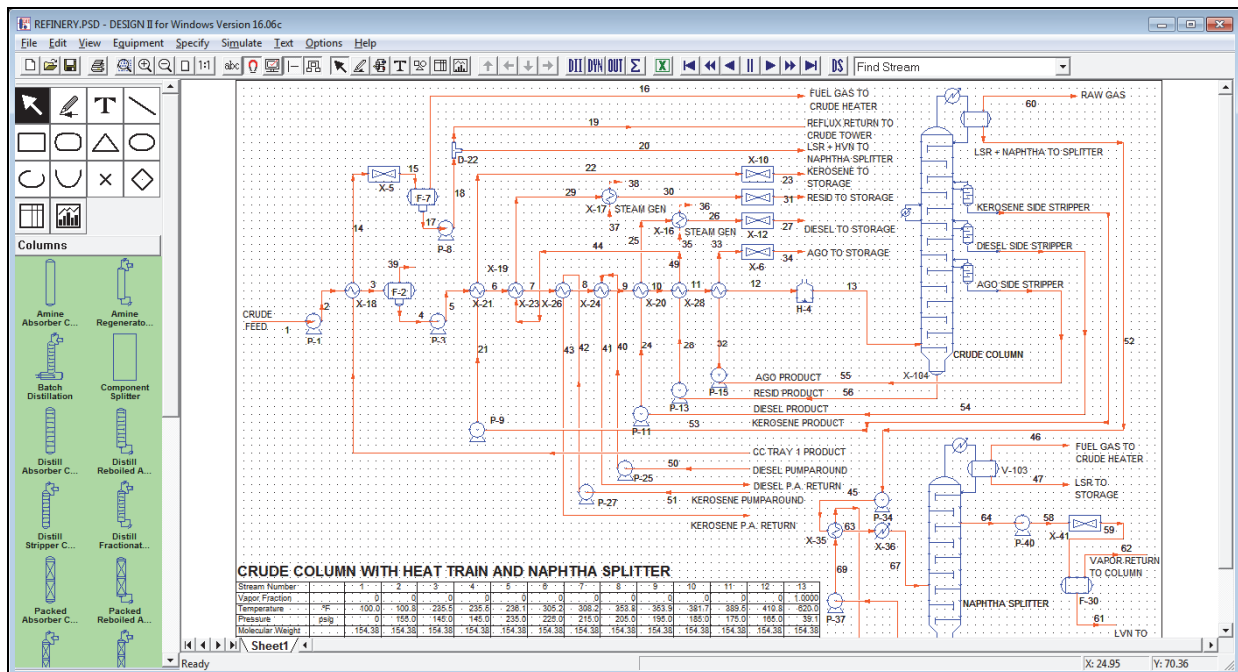


# DESIGN II<sup>TM</sup> ChemTran<sup>TM</sup>

## General Reference Guide Version 16.0



**WinSim<sup>®</sup> Inc.**  
*Advanced Engineering Software*

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# TABLE OF CONTENTS

<b>CHAPTER 1: INTRODUCTION .....</b>	<b>1</b>
EXECUTING DESIGN II FILES VIA THE COMMAND LINE .....	1
INPUT COMMANDS .....	1
INPUT SECTIONS .....	2
INPUT GUIDELINES .....	2
ENTERING NUMERICAL QUANTITIES .....	3
ENTERING EQUIPMENT MODULES .....	3
ENTERING DIMENSIONAL UNITS .....	3
ENTERING COMMENTS .....	4
SAMPLE DESIGN II OUTPUT .....	4
EXAMPLE FLOWSHEET SIMULATION-DEBUTANIZER COLUMN DESIGN .....	10
DESIGN II LIMITATIONS .....	10
<b>CHAPTER 2: DATABASE COMPONENTS .....</b>	<b>11</b>
COMPONENT DATABASE SORTED BY ID .....	11
COMPONENT DATABASE - ID FROM 1 TO 99 .....	11
COMPONENT DATABASE - ID FROM 100 TO 999 .....	13
COMPONENT DATABASE - ID FROM 1000 TO 1999 .....	13
COMPONENT DATABASE - ID FROM 2000 TO 2999 .....	32
COMPONENT DATABASE - ID FROM 3000 TO 3999 .....	34
COMPONENT DATABASE - ID FROM 4000 TO 4999 .....	39
COMPONENT DATABASE - ID FROM 5000 TO 5999 .....	44
COMPONENT DATABASE - ID FROM 6000 TO 6999 .....	45
COMPONENT DATABASE - ID FROM 7000 TO 7999 .....	45
COMPONENT DATABASE - ID FROM 8000 TO 8999 .....	46
COMPONENT DATABASE - ID FROM 9000 TO 9999 .....	48
COMPONENT DATABASE FOR MIXED AMINE .....	49
COMPONENT PROPERTIES STORED .....	50
COMPONENT PROPERTIES ESTIMATION METHODS .....	51
DESIGN II IONIC COMPONENT LIBRARY .....	51
<b>CHAPTER 3: SPECIFYING FEED STREAMS .....</b>	<b>53</b>
REAL FEEDS COMMAND DETAILS .....	53
REAL FEEDS COMMAND SUMMARY .....	55
REAL FEEDS STREAM PHASE SPECIFICATION .....	55
REAL FEEDS HEATING VALUE COMMANDS .....	55
PETROLEUM (PSEUDO) FRACTIONS .....	56
PETROLEUM FRACTION ESSENTIAL COMMANDS .....	56
PETROLEUM FRACTION OPTIONAL COMMANDS .....	57
FEEDS THERMODYNAMIC OPTIONAL COMMAND .....	58
SPECIFYING AND REFERENCING A FEED STREAM .....	59
<b>CHAPTER 4: CRUDE BULK FEED STREAMS .....</b>	<b>61</b>
CRUDE BULK FEED COMMAND DETAILS .....	61
CRUDE BULK FEED OPTIONAL PROPERTIES .....	65
CRUDE BULK FEED STEP BY STEP .....	68
<b>CHAPTER 5: COMPONENT BY COMPONENT CRUDE STREAMS .....</b>	<b>71</b>
COMPONENT BY COMPONENT COMMAND DETAILS .....	71
COMPONENT BY COMPONENT OPTIONAL COMMANDS .....	72
COMPONENT BY COMPONENT CRUDE FEED COMMAND SUMMARY .....	74
COMPONENT BY COMPONENT EXAMPLES .....	74
<b>CHAPTER 6: CRUDE OIL LIBRARY .....</b>	<b>79</b>
CRUDE OIL LIBRARY TABLE .....	79
CRUDE OIL LIBRARY COMMAND DETAILS .....	79
CRUDE OIL LIBRARY COMMAND SUMMARY .....	80
CRUDE OIL LIBRARY EXAMPLE .....	80
<b>CHAPTER 7: THERMODYNAMICS .....</b>	<b>81</b>
THERMODYNAMICS: K-VALUE OPTIONS .....	81

THERMODYNAMICS: ENTHALPY OPTIONS .....	88
THERMODYNAMICS: DENSITY OPTIONS .....	91
THERMODYNAMICS: TRANSPORT PROPERTY OPTIONS.....	94
THERMODYNAMICS: MIXED AMINE .....	97
THERMODYNAMICS: PURE COMPONENT PROPERTY COMMANDS .....	98
THERMODYNAMICS: PROPERTY COMMAND SUMMARY .....	101
THERMODYNAMICS: STEP BY STEP .....	102
THERMODYNAMICS: NOTES.....	105
THERMODYNAMICS: UNIFAC AND LLE UNIFAC SPECIFICATION EXAMPLE .....	124
THERMODYNAMICS: REFERENCES.....	125
<b>CHAPTER 8: CALCULATION OPTIONS.....</b>	<b>131</b>
CALCULATION OPTIONS IN FLOWSHEET .....	131
CALCULATION OPTIONS COMMAND SUMMARY .....	135
CALCULATION OPTIONS STEP BY STEP .....	136
CALCULATION OPTIONS EXAMPLES.....	137
<b>CHAPTER 9: PRINT OPTIONS.....</b>	<b>145</b>
PRINT OPTIONS GENERAL .....	145
PRINT OPTIONS COMMAND SUMMARY .....	147
PRINT OPTIONS STEP BY STEP .....	148
PRINT OPTIONS EXAMPLES.....	148
<b>CHAPTER 10: RECYCLE LOOPS .....</b>	<b>153</b>
RECYCLE LOOPS INITIAL GUESSES .....	153
RECYCLE LOOPS CALCULATION OPTIONS.....	153
RECYCLE LOOPS PRINT OPTIONS.....	157
RECYCLE LOOPS REVERSE CALCULATION .....	157
RECYCLE LOOPS COMMAND SUMMARY .....	158
RECYCLE LOOPS STEP BY STEP .....	158
RECYCLE LOOPS MINIMIZING CALCULATIONS.....	159
RECYCLE LOOPS REVIEW OF DESIGN II OUTPUT .....	161
RECYCLE LOOPS EXAMPLE USING CASE STUDY REPEAT COMMAND .....	162
<b>CHAPTER 11: INPUT UNITS .....</b>	<b>165</b>
INPUT UNITS: KEYWORD UNIT SPECIFICATION .....	165
INPUT UNITS: INDIVIDUAL QUANTITY UNIT SPECIFICATION.....	165
INPUT UNITS: COMMAND SUMMARY .....	165
INPUT UNITS: STEP BY STEP .....	165
INPUT UNITS: GLOBAL UNIT SPECIFICATION .....	166
INPUT UNITS: (DEFAULT) FOR GLOBAL SYSTEMS .....	166
INPUT UNITS: OPTIONS.....	167
INPUT UNITS: EXAMPLES.....	168
<b>CHAPTER 12: OUTPUT UNITS .....</b>	<b>169</b>
OUTPUT UNITS: INDIVIDUAL OUTPUT QUANTITY UNIT SPECIFICATION.....	169
OUTPUT UNITS: GLOBAL OUTPUT UNIT SPECIFICATION.....	170
OUTPUT UNITS: COMMAND SUMMARY.....	170
OUTPUT UNITS: STEP BY STEP.....	170
OUTPUT UNITS: EXAMPLES .....	171
OUTPUT UNITS: OPTIONS .....	172
OUTPUT UNITS: BY SYSTEM.....	173
<b>CHAPTER 13: STREAM FILES.....</b>	<b>175</b>
STREAM FILES STEP BY STEP.....	175
<b>CHAPTER 14: SAVING STREAM DATA.....</b>	<b>177</b>
<b>CHAPTER 15: CASE STUDY.....</b>	<b>179</b>
CASE STUDY COMMAND DETAILS .....	179
CASE STUDY FORMAT SECTION.....	179
CASE STUDY EXAMPLES .....	180
CASE STUDY SAMPLES.....	180
<b>CHAPTER 16: CHEMTRAN .....</b>	<b>181</b>
CHEMTRAN OVERVIEW.....	181
CHEMTRAN FILES AND DATA LIBRARIES.....	184

CHEMTRAN ENTERING DATA .....	185
CHEMTRAN FILE ACCESS COMMANDS .....	185
CHEMTRAN DESIGN II INTERFACE .....	186
CHEMTRAN ELECTROLYTE (IONIC) COMPONENT DATA ENTRY .....	187
CHEMTRAN CORRELATING MIXTURE DATA .....	190
CHEMTRAN: MIXTURE COMMAND DETAILS .....	196
CHEMTRAN PURE COMPONENT COMMAND DETAILS .....	214
CHEMTRAN: COMPONENT PROPERTIES COMMAND DETAILS .....	217
CHEMTRAN PURE COMPONENT PROPERTY GENERATION .....	231
CHEMTRAN: PURE COMPONENT OPTIONAL COMMANDS .....	244
CHEMTRAN STEP BY STEP .....	251
CHEMTRAN EXAMPLES .....	253
CHEMTRAN REFERENCES .....	259
<b>CHAPTER 17: FLOWSHEET OPTIMIZATION .....</b>	<b>261</b>
FLOWSHEET OPTIMIZATION OVERVIEW .....	261
FLOWSHEET OPTIMIZATION COMMAND DETAILS .....	261
FLOWSHEET OPTIMIZATION GUIDELINES .....	264
FLOWSHEET OPTIMIZATION REFERENCE TABLES .....	267
FLOWSHEET OPTIMIZATION EXAMPLES .....	269
FLOWSHEET OPTIMIZATION REFERENCE .....	269
<b>CHAPTER 18: INLINE FORTRAN .....</b>	<b>271</b>
INLINE FORTRAN OVERVIEW .....	271
INLINE FORTRAN COMMAND DETAILS .....	271
INLINE FORTRAN GUIDELINES .....	276
INLINE FORTRAN PARAMETERS, MODULE FUNCTIONS, AND PROPERTY BANKS .....	280
INLINE FORTRAN OPERATORS, FUNCTIONS, AND KEYWORDS .....	282
INLINE FORTRAN EXAMPLES .....	284
INLINE FORTRAN: TABLE 1. INLINE FORTRAN RESTRICTIONS .....	284
INLINE FORTRAN: TABLE 2. VARIABLES AVAILABLE TO GET AND SET .....	285
INLINE FORTRAN: TABLE 3. DISTILLATION FUNCTION .....	292
INLINE FORTRAN: TABLE 4. COMPONENT PROPERTIES (Tc,Pc,..) SUBROUTINES .....	292
INLINE FORTRAN: TABLE 5. UTILITIES SUBROUTINE (USE WITH CALL) .....	293
INLINE FORTRAN: TABLE 6. THERMODYNAMIC LIBRARY SUBROUTINES (USE WITH CALL) .....	293
INLINE FORTRAN: TABLE 7. THERMODYNAMIC INTERACTION PARAMETERS .....	294
INLINE FORTRAN: TABLE 8. DESIGN II FLASH SUBROUTINE (USE WITH CALL) .....	298
INLINE FORTRAN: TABLE 9. REFINE MODULE SUBROUTINES .....	299
<b>CHAPTER 19: INTERACTIVE PROCESSING .....</b>	<b>301</b>
INTERACTIVE PROCESSING OVERVIEW .....	301
INTERACTIVE PROCESSING COMMAND DETAILS .....	301
INTERACTIVE PROCESSING UNITS MENU .....	301
INTERACTIVE PROCESSING SCROLL COMMANDS .....	302
INTERACTIVE PROCESSING EXAMPLE .....	302
<b>CHAPTER 20: SIZE LINES .....</b>	<b>309</b>
SIZE LINES OVERVIEW .....	309
SIZE LINES COMMAND DETAILS .....	310
SIZE LINES OPTIONAL COMMAND DETAILS .....	310
SIZE LINES COMMAND SUMMARY .....	313
SIZE LINES STEP BY STEP .....	313
SIZE LINES EXAMPLES .....	314
SIZE LINE REFERENCES .....	315



# Chapter 1: Introduction

In addition to rigorous heat and material balance calculations, DESIGN II also offers advanced features such as equipment rating and sizing calculations in the flowsheet. For example, DESIGN II performs heat exchanger rating, pipeline modeling, distillation tray sizing/rating, vessel sizing, and more.

For added flexibility Inline FORTRAN allows you to easily add your own calculations by simply adding FORTRAN statements directly in the input file. Inline FORTRAN gives you access to flowsheet variables and even to DESIGN II's library of routines for thermodynamic and physical properties.

A powerful optimization feature allows you to define your objective and DESIGN II automatically finds the optimum. The objective function can be a simple function of flowsheet parameters or a complex economic function defined directly with Inline FORTRAN.

## Executing DESIGN II Files Via the Command Line

To run DESIGN II from the command line, type the following command: `des filename (no extension)`

DESIGN II will read the file `filename.in` and write (create) the output file `filename.out`.

You can directly execute DESIGN II by: `designii.exe filename.in filename.out`

## Input Commands

DESIGN II uses an ASCII input file which can be created or read with any text editor. DESIGN II for Windows creates this input file every time DESIGN II is executed.

The first line of the input file is the DESIGN II account number. The DESIGN II account number is obsolete but is maintained.

Specifications and calculation information are presented to the program in the form of commands, all of which are described in this Guide. A typical input file is shown below. This input is from the example simulation explained in detail in Flowsheet Procedure: Example Flowsheet Simulation-Debutanizer Column Design.

DESIGN II Account Number	<b>AB123.</b>
Title	*DEBUTANIZER DESIGN
	<b>HEAT EXCHANGER 1 = OVHD, 4,1, -6, -2</b>
	<b>TEMPERATURE APPROACH = 10</b>
Equipment	<b>HEAT EXCHANGER 2 = BOTS, 5, 2, -7, -3</b>
Module	<b>TEMPERATURE APPROACH = 20</b>
Commands	<b>SHORTCUT FRACTIONATOR 3 = DEC4, 3, -4, -5</b>
	<b>PRESSURE TOP =200, RECOVER TOP 6 =.98</b>
	<b>RECOVER BOTTOM 7 = .95</b>
	<b>PARTIAL CONDENSER</b>
	<b>GENERAL</b>
	<b>COMPONENTS = 4, 5, 6, 7, 8, 10, 100</b>
	<b>API 100 = 40, AMB 100 = 350</b>
	<b>AMW 100 = 136</b>
GENeral	<b>NAME 100 = C7+</b>
Commands	<b>TP1 = 80,210</b>
	<b>FLOW 1= 2000, 400, 600, 150.3, 200, 50.8, 250</b>
END Command	<b>END</b>

The boldface characters represent the *keywords* which are recognized by the program and which must be entered. If you wish, you can enter only the keywords for each command, thereby reducing the amount of input. The same input information would then look like this:

```
AB123.
*DEBUTANIZER DESIGN
HEA EXC 1 = OVHD, 4, 1, -6, -2,
TEM APP = 10
HEA EXC 2 = BOTS, 5, 2, -7, -3,
TEM APP = 20
SHO 3 = DEC4, 3, -4, -5, PRE TOP = 200
REC TOP 6 = .98, REC BOT 7 = .95,
PAR
GEN,
COM = 4, 5, 6, 7, 8, 10, 100, API 100 = 40
AMB 100 = 350, AMW 100 = 136, NAM 100 = C7+
TP 1 = 80, 210, FLO 1 = 2000, 400, 600, 150.3,200, 50.8, 250
END
```

## Input Sections

A DESIGN II input file is organized into sections. Each section begins with one of the keywords in the figure below, such as **HEA EXC** and **GEN**. All the commands that apply to one section are entered after that section keyword but before the next section keyword. Thus, in the example above, all the shortcut fractionator commands are entered after the keyword SHO but before the next section keyword GENERAL.

1. Design II Account Number	<b>AB123.</b>
2. Title	<b>* title here</b>
3. Equipment modules for example	<i>equipment modules here</i>
4. General section	<b>HEA EXC 1 = OVHD, 4,1,-6,-2</b>
5. Crude section	<b>GEN</b>
6. Size lines section	<b>CRU</b>
7. Optimization section	<b>SIZ LIN</b>
8. Inline FORTRAN section	<b>OPTIM</b>
9. END command	<b>FORTRAN</b>
	<b>END</b>

### Order of Input

The only restriction on the order of sections is that the account number must always be first, the title second and the END command last. The other sections can be in any order and can be repeated any number of times.

### DESIGN II Account Number

Your DESIGN II account number by default is **AB123.** and will always be in the first line of the input. The trailing period must be included as part of the account.

### Program Defaults

Many Equipment Module and GENeral commands are optional in DESIGN II. If you choose not to enter such commands, the program automatically defaults to a standard value or specification. Defaults are given in the descriptions for optional commands. You should evaluate the defaults to determine if they are suitable for your simulations. If they are not, you should use the commands to enter your own values or specifications.

In addition, if you do not specify the units for the data you enter, the program automatically uses the standard default units presented in *Input/Output Units*. If your data is in other units, be sure to specify them as explained in that section of the Guide.

## Input Guidelines

### Margins

Each line of input may begin at the left margin and continue to the right for 80 characters and spaces. The Title, END, GENeral, and Comment commands, as well as Equipment Module identifiers usually begin at the left margin, since each must be the first command on the line. The program reads a maximum of 80 characters per line.

### Blank Spaces Allowed

You can use as many blank spaces as you wish. No blank spaces are required in the input, although the spacing illustrated in the example makes it easier to review the input.

### Where to Break Lines

You can enter as many commands as you like on a single line (within the margin limits), but a command cannot be broken and continued on the next line. Lines of input can be continued on another line and no special continuation character or signal is required. For example,

Wrong: **HEA EXC 1 = OVHD, 4, 1, -6, -2, TEM**  
**APP =10**

Wrong: **HEA EXC = OVHD, 4, 1, -6, -2, TEM APP =10**

Wrong: **HEA EXC 1 =OVHD, 4, 1, -6, -2, TEM APP = 10**

Right: **HEA EXC 1 = OVHD, 4, 1, -6, -2 TEM APP = 10**

Right: **HEA EXC 1 = OVHD, 4, 1, -6, -2,**  
**TEM APP =10**

Numerals following a command (for example, component flowrates) can be continued on the next line or lines, but a number cannot be broken:

Wrong: **FLO 1 = 2000, 400, 600, 150.3, 2**  
**00, 50.8, 250**

Right: **FLO 1 = 2000, 400, 600, 150.3**  
**200, 50.8, 250**

Commas are required to separate commands and data entries, but no comma is needed at the end of a line unless the line



extends beyond column 70.

### Blank Lines Are Allowed

You can include blank lines anywhere after the Design II account number for clarity and readability of input.

### Minimum Keyword Input

Each command may be abbreviated to the minimum letters shown boldfaced in this manual, usually the first three letters of each word:

Right:	FLASH
Right:	FLAS
Right:	FLA
Right:	HEAT EXCHANGER
Right:	HEAT EXCH
Right:	HEA EXC

### Inline FORTRAN

FORTRAN statements can be entered with any equipment module, see *Inline FORTRAN*. These FORTRAN statements require **F-** in columns one and two, six blank spaces, then the statement as shown below:

```
F-      DEL= 15.5 + FLOW*(TEM**2)
```

## Entering Numerical Quantities

### Commas

Never use commas to indicate order of magnitude; commas are used only to separate commands and data entries on the same line:

Wrong:	<b>FLO</b> 1 = 2,000, 400, 600
Right:	<b>FLO</b> 1 = 2000, 400, 600

### Decimals

When no decimal is entered, the program automatically places one to the right of the last digit. For example, if you enter 100, it is assumed to be 100.0 by the program.

### Scientific Notation

Exponential values can be entered using scientific notation. For example, 8,500,000 (8.5 x 10<sup>6</sup>) is entered as 8.5E6.

### Repetitive Numbers

When you are entering a series of identical values, you can shorten the entry with the use of asterisk notation as follows:

Instead of:	<b>FLO</b> 1 = 150, 150, 150, 150, 150, 150,
Enter:	<b>FLO</b> 1 = 6*150

## Entering Equipment Modules

Equipment Module sections typically follow the Title command. All equipment module sections begin with a line in the following format:

format:	<b>equipment identifier number = n, input streams, -output streams</b>
example:	<b>HEA EXC 1 =</b> OVHD, 4, 1, -6, -2,
where:	<b>HEA EXC 1</b> is the DESIGN II equipment module identifier and "1" is the assigned equipment number.
	OVHD is your descriptive name for the module.
	4, 1 are the input streams to the module
	-6, -2 are the output streams from the module

This line defines the connections of units and streams on the flowsheet. Each equipment in the flowsheet is given a unique number from 1 to 999. Each stream is also given a unique number from 1 to 999. A stream and an equipment can have the same number but no two equipment can have the same number and no two streams can have the same number. Input streams to equipment are always positive integers while output streams are always negative integers.

## Entering Dimensional Units

Most DESIGN II specifications can be entered in any dimensional units.

See *Input/Output Units* for details.

Unit options are available for most input commands. Alternatively, you can use one of the overall unit option commands to

# Chapter 1

choose a specific set of unit options which are to be used for both input and output. Alternate unit options can be specified within a set. See *Input/Output Units* for details.

If you wanted all your input and output to be in metric units, you would enter the following commands in the GENERAL section of your input file:

```
METRIC UNITS
```

Suppose you preferred to have the pressure units in the output in bars, rather than KG/CM2. You would add a command as follows:

```
MET UNI, PRE UNI OUT = BAR
```

## Entering Comments

A special Comments command can be used for self-documentation. This command can be inserted anywhere in the input and allows you to make notes or remarks as you wish.

To use this feature, simply enter **C-** starting at the left margin, and then enter your comment. For example:

```
C- THIS EXCHANGER SETS THE APPROACH
C- TEMPERATURE BETWEEN STREAMS 1 AND 6
HEA EXC 1 = OVHD, 4, 1, -6, -2,
TEM APP =10
```

## Sample DESIGN II Output

The printout information for all DESIGN II simulations is presented in basically the same format. The following discussion examines the sample problem initial run printout.

### Page 1 of Printout

The second printout page presents an exact duplicate (echo print) of your input data as read by DESIGN II, including blank lines and spaces between commands. For security reasons, your DESIGN II account number does not appear.

Error messages are printed when there are misspelled or incorrect commands or when there are syntax errors in your input coding. When error messages occur, review your input carefully and make all necessary corrections.

```
ECHO PRINT OF INPUT DATA
*DEBUTANIZER DESIGN
HEA EXC 1 = OVHD, 4,1,-6,-2,TEM APP = 10
HEA EXC 2 = BOTS, 5,2,-7,-3,TEM APP = 20
SHO 3 = DEC 4,3,-4,-5,PRE TOP = 200
      REC TOP 6 =.98,REC BOT 7 = .95, PAR
GEN
      COM = 4,5,6,7,8,10,100
      API 100 = 40,AMB 100 = 350,AMW 100 = 136, MAX=10
      NAM 100 = C7+
      TP1 = 80,210
      FLO1 = 2000,400,600,150.3,200,50.8,250
END
```

### Page 2 of Printout

Page 3 lists all streams for which TP and FLOW commands were entered and product streams. This list allows you to check the flowsheet carefully to make sure no stream numbers were miscoded and that DESIGN II sees the same flowsheet you do.

```
STREAM THERMODYNAMIC INITIALIZATION
```

STREAM NUMBER	KVALUES	ENTHALPIES	DENSITY
-----	-----	-----	-----
1	STD	STD	STD

```
THE FOLLOWING STREAMS ARE FEED STREAMS TO THE PROCESS
```

```
STREAM NUMBER
-----
1
```

```
THE FOLLOWING STREAMS ARE PRODUCT STREAMS FROM THE PROCESS
```

```
STREAM NUMBER
-----
6
7
```

### Page 3 of Printout

#### Section A

The name of each component listed in the COMponents command is printed along with its ID number. Verify that the

components are the ones you want.

```

++SYSTEM VARIABLES++
-----
NUMBER OF COMPONENTS      7

COMPONENTS USED...      4  PROPANE
                        5  I-BUTANE
                        6  N-BUTANE
                        7  I-PENTANE
                        8  N-PENTANE
                       10  N-HEXANE
                       100 C7+

ENTHALPY DATUM IS IDEAL GAS AT 32 DEGREES F
ENERGY SIGN CONVENTION: WORK PRODUCED BY THE EQUIPMENT IS POSITIVE
                        HEAT TRANSFERRED TO THE EQUIPMENT IS POSITIVE
STANDARD CONDITIONS ARE STP 60.00 DEG F AND 14.696 PSIA
                        NTP  0.00 DEG C AND  1.00 ATM
                        API  15.00 DEG C AND  1.00 ATM
LIQUID GAL AND BBL ARE U.S. GAL AND BBL

```

### Section B

This section is important only if the simulation contains a recycle condition. The default CONvergence TOLerance (.001) represents a 0.1% error in heat and material balance. If you think a less stringent error will be sufficient, add a **CON TOL = .01** command anywhere in the GENERAL command section of your input. See *Recycle Loops* for details.

```

RECYCLE LOOP CONVERGENCE TOLERANCE      0.0010

MAXIMUM RECYCLE LOOPS                    1
AUTOMATIC RECYCLE CALC. SEQUENCE USED

```

### Section C

This section tells you which K-value and enthalpy correlations will be used. If no K-value or enthalpy options were selected, the default correlations are shown and used in the calculations. To change these options, see Thermodynamics Section.

```

++++++ GENERAL THERMOPHYSICAL PROPERTY OPTIONS ++++++

```

```

KVALUES      ENTHALPIES      DENSITIES      VAPOR FUGACITIES
=====
STD          STD            STD            STD VAP
=====
          VISCOSITY          THERMAL CONDUCTIVITY
          -----          -----
LIQUID      VAPOR          LIQUID      VAPOR
=====
NBS81       NBS81          NBS81       NBS81
=====

SURFACE TENSION
=====
STD

```

```

++++++ PETROLEUM FRACTION PROPERTY OPTIONS ++++++

```

```

MOLECULAR WT      CRITICAL TEMP      CRITICAL PRES
=====
CAVETT           CAVETT           CAVETT

```

### Page 5 of Printout

The message BEGIN RECYCLE LOOP 1 indicates a recycle situation. All equipment listed just before the END RECYCLE LOOP 1 message are contained in the recycle loop.

The message RECYCLE STREAM = 3 means that the program requires initial **TP** and **FLOW** guesses for stream 3. These parameters will then be adjusted until convergence occurs.

The equipment in the recycle loop are listed in the calculation order, unless a **RECYCLE SEQUENCE** command is added to the GENERAL command section.

**NOTE:** If you look at the example problem flowsheet, you will see that stream 3 is not a true recycle stream, but the program has determined that it is the only stream needed to solve the problem. This saves time and money, since only one stream, not two, requires a guess. Also, since stream 3 is the same as the feed (stream 1), only the temperature must be guessed (the moles of stream 3 must still be entered as initial guess with a **FLOW 3 =** command). The problem is solved much faster because acceleration and convergence are performed on only one stream.

```

+++++UNIT CALCULATION SEQUENCE ANALYSIS

E Q U I P M E N T

```

# Chapter 1

```

INLET STREAMS          TYPE NUMBER NAME          OUTLET STREAMS
-----
*****BEGIN RECYCLE LOOP 1*****
*****RECYCLE STREAM = 3 CONNECTING FROM ( 2) BOTS
                        TO ( 3) DEC 4
    3          SHO          3 DEC 4          4 5
    4 1        HEAEXC       1 OVHD          6 2
    5 2        HEAEXC       2 BOTS          7 3
*****END RECYCLE LOOP 1

```

## Page 8 of Printout

RESULTS FROM SHORT CUT FRACTIONATION  
FOR A PARTIAL CONDENSER

+++DISTILLATE VAPOR PRODUCT+++

	LBMOL/HR	MOL PERCENT	LB/HR
1 PROPANE	2000.0	66.745	88188.
2 I-BUTANE	399.12	13.320	23197.
3 N-BUTANE	588.00	19.623	34175.
4 I-PENTANE	7.5150	0.25079	542.18
5 N-PENTANE	1.8626	6.21596E-02	134.38
6 N-HEXANE	1.02554E-04	3.42246E-06	8.83726E-03
7 C7+	2.50000E-07	8.34308E-09	3.40000E-05
TOTALS	2996.5	100.00	1.46236E+05

TEMPERATURE DEG F 143.03  
PRESSURE PSIA 200.00  
ENTHALPY BTU/HR 4.48373E+06  
MOLECULAR WT 48.802

+++BOTTOM PRODUCT+++

	LBMOL/HR	MOL PERCENT	LB/HR
1 PROPANE	1.70898E-03	2.61071E-04	7.53560E-02
2 I-BUTANE	0.88159	0.13468	51.238
3 N-BUTANE	12.000	1.8332	697.44
4 I-PENTANE	142.79	21.812	10301.
5 N-PENTANE	198.14	30.268	14295.
6 N-HEXANE	50.800	7.7604	4377.5
7 C7+	250.00	38.191	34000.
TOTALS	654.61	100.00	63722.

TEMPERATURE DEG F 344.40  
PRESSURE PSIA 200.00  
ENTHALPY BTU/HR 1.69173E+06  
MOLECULAR WT 97.345

+++COLUMN PARAMETERS BY SHORT CUT METHOD+++

% OF MIN REFLUX	REFLUX RATIO	STAGES	FEED TRAY LOCATION	CONDENSER DUTY BTU/HR	REBOILER DUTY BTU/HR
105.0	0.757	58.43	31.88	0.1390E+08	0.7021E+07
110.0	0.793	41.99	22.75	0.1456E+08	0.7682E+07
120.0	0.865	30.71	16.49	0.1588E+08	0.9006E+07
140.0	1.009	23.21	12.33	0.1853E+08	0.1165E+08
175.0	1.262	18.87	9.92	0.2316E+08	0.1629E+08
200.0	1.442	17.50	9.16	0.2647E+08	0.1960E+08
130.0	0.937	25.93	13.84	0.1721E+08	0.1033E+08

Thermodynamics options used in each Equipment Module are reported along with the calculation time in seconds.

NOW CALLING EQUIPMENT 1 + HEAEXC = OVHD  
KVALUES - STD ENTHALPY - STD DENSITY - STD

## Page 15 of Final Run Printout

The example simulation converged after three iterations through the equipment calculations.

\*\*\*\*LOOP 1 HAS CONVERGED AFTER 3 ITERATIONS\*\*\*\*

## Pages 17 and 18 of Final Run Printout

Properties of each stream in the process are printed in the final Stream Summaries

## STREAM SUMMARY

STREAM NUMBER	1	2	3	4
STREAM NAME				
EQUIP CONXION	FEED-OVHD ( 0)-( 1)	OVHD-BOTS ( 1)-( 2)	BOTS-DEC ( 2)-( 3)	DEC -OVHD ( 3)-( 1)
VAPOR FRACTION	0.00000E+00	0.00000E+00	0.21542	1.0000
TEMPERATURE F	80.000	133.03	153.78	143.03
PRESSURE PSIA	210.00	210.00	210.00	200.00
ENTHALPY BTU/HR	-0.27166E+08	-0.20356E+08	-0.13121E+08	0.44837E+07
V Cp BTU/LBMOL/R			24.071	24.354
V Cv BTU/LBMOL/R			19.685	19.809
L Cp BTU/LBMOL/R	34.378	36.155	38.038	
V DEN LB/FT3			1.9058	1.9019
L DEN LB/FT3	35.142	32.686	32.540	
L S.G. (60F) STP	0.57885	0.57885	0.59126	
V VIS CP			0.99282E-02	0.96844E-02
L VIS CP	0.15346	0.11663	0.11498	
V THC BTU/FT/HR/F			0.14662E-01	0.14106E-01
L THC BTU/FT/HR/F	0.63455E-01	0.56260E-01	0.55093E-01	
V MMSCF/DAY STP			7.1624	27.287
L GAL/MIN STP	725.10	725.10	582.42	
TOTAL MOLE WEIGHT	57.505	57.505	57.505	48.802

L-LIQUID PHASE (EXCLUDING IMMISCIBLE WATER), V-VAPOR PHASE  
Cp,Cv-HEAT CAPACITY, DEN-DENSITY, VIS-VISCOSITY, THC-THERMAL CONDUCTIVITY

## FLOW RATES LBMOL/HR

PROPANE	2000.0	2000.0	2000.0	2000.0
I-BUTANE	400.00	400.00	400.00	399.12
N-BUTANE	600.00	600.00	600.00	588.00
I-PENTANE	150.30	150.30	150.30	7.5150
N-PENTANE	200.00	200.00	200.00	1.8626
N-HEXANE	50.800	50.800	50.800	0.10255E-03
C7+	250.00	250.00	250.00	0.25000E-06
TOTAL LBMOL/HR	3651.1	3651.1	3651.1	2996.5
TOTAL LB/HR	0.20996E+06	0.20996E+06	0.20996E+06	0.14624E+06

## STREAM SUMMARY (CONTINUED)

STREAM NUMBER	5	6	7
STREAM NAME			
EQUIP CONXION	DEC -BOTS ( 3)-( 2)	OVHD-PROD ( 1)-( 0)	BOTS-PROD ( 2)-( 0)
VAPOR FRACTION	0.00000E+00	0.65609	0.00000E+00
TEMPERATURE F	344.40	136.00	153.03
PRESSURE PSIA	200.00	200.00	200.00
ENTHALPY BTU/HR	0.16917E+07	-0.23262E+07	-0.55434E+07
V Cp BTU/LBMOL/R		23.731	
V Cv BTU/LBMOL/R		19.192	
L Cp BTU/LBMOL/R	63.030	34.643	53.687
V DEN LB/FT3		1.8868	
L DEN LB/FT3	34.946	29.624	42.288
L S.G. (60F) STP	0.72229	0.54200	0.72229
V VIS CP		0.96294E-02	
L VIS CP	0.12703	0.85095E-01	0.29612
V THC BTU/FT/HR/F		0.13950E-01	
L THC BTU/FT/HR/F	0.50426E-01	0.50134E-01	0.66436E-01
V MMSCF/DAY STP		17.903	
L GAL/MIN STP	176.36	192.33	176.36
TOTAL MOLE WEIGHT	97.345	48.802	97.345

L-LIQUID PHASE (EXCLUDING IMMISCIBLE WATER), V-VAPOR PHASE  
Cp,Cv-HEAT CAPACITY, DEN-DENSITY, VIS-VISCOSITY, THC-THERMAL CONDUCTIVITY

## FLOW RATES LBMOL/HR

PROPANE	0.17090E-02	2000.0	0.17090E-02
I-BUTANE	0.88159	399.12	0.88159
N-BUTANE	12.000	588.00	12.000
I-PENTANE	142.79	7.5150	142.79
N-PENTANE	198.14	1.8626	198.14
N-HEXANE	50.800	0.10255E-03	50.800
C7+	250.00	0.25000E-06	250.00

# Chapter 1

```

TOTAL      LBMOL/HR      654.61      2996.5      654.61
TOTAL      LB/HR          63722.      0.14624E+06 63722.
    
```

## Page 21 of Final Run Printout

Minimum reflux and stages, feed tray locations, reflux ratio, number of theoretical stages, and condenser and reboiler duty results are reported for the specified PERcent of MINimum reflux. For this example, the default value of 130 is used for percent of minimum reflux since a PER MIN command was not entered.

\*\*\*\*SHORTCUT DISTILLATON\*\*\*\*

```

EQUIPMENT NO.          3

EXTERNAL NAME          DEC 4
LIGHT KEY ID NO.       6
FRAC. LIGHT KEY
OVERHEAD               0.98000
HEAVY KEY ID NO.      7
FRAC. HEAVY KEY
BOTTOM                0.95000
COL. PRES. DROP
PSI                   0.00000E+00
PCT MIN REFLUX        130.00
OVERHEAD PHASE
0= VAPOR
1= LIQUID             0.00000E+00
MINIMUM REFLUX        0.63738
MINIMUM STAGES        12.725
FEED TRAY FR TOP      14.232
REFLUX RATIO          0.82859
NO. OF STAGES         26.642
CONDENSER DUTY
BTU/HR                -1.52121E+07
REBOILER DUTY
BTU/HR                3.45086E+07
    
```

## Page 22 of Final Run Printout

The Material Balance Summary shows the mole balance for every component in the simulation. In this example there was an iterative recycle calculation. The balance shows that indeed the flowsheet did converge and that all components are in material balance.

### M A T E R I A L B A L A N C E S U M M A R Y

COMPONENT NAME	FEED(S) LBMOL	PRODUCT(S) LBMOL	DIFFERENCE LBMOL	REL. ERROR
PROPANE	2000.	2000.	0.0000E+00	0.0000E+00
I-BUTANE	400.0	400.0	0.0000E+00	0.0000E+00
N-BUTANE	600.0	600.0	0.0000E+00	0.0000E+00
I-PENTANE	150.3	150.3	0.0000E+00	0.0000E+00
N-PENTANE	200.0	200.0	0.0000E+00	0.0000E+00
N-HEXANE	50.80	50.80	0.0000E+00	0.0000E+00
C7+	250.0	250.0	0.0000E+00	0.0000E+00
TOTAL	3651.	3651.	0.0000E+00	0.0000E+00
FLOWRATE /HR				

## Page 23 of Final Run Printout

One detailed stream printout page is printed for each stream which is calculated and contains moles. The detailed stream summary page is where transport properties, critical properties, or other mixture properties will be printed, if requested.

```

STREAM NUMBER      1      CONNECTING ( 0) FEED
                     TO      ( 1) OVHD
STD K-VALUES      STD ENTHALPY      STD DENSITY      FLOW RATES /HR

COMPONENT NAME      TOTAL LIQUID VAPOR      TOTAL TOTAL
                     LBMOL  LBMOL  LBMOL      LB    MOL PCT  KVALUE
-----
PROPANE              2000.00 2000.00      0.  88188.0  54.778
I-BUTANE              400.000 400.000      0.  23248.0  10.956
N-BUTANE              600.000 600.000      0.  34872.0  16.433
I-PENTANE             150.300 150.300      0.  10843.5  4.1166
N-PENTANE             200.000 200.000      0.  14429.2  5.4778
N-HEXANE              50.8000 50.8000      0.  4377.54  1.3914
C7+                   250.000 250.000      0.  34000.0  6.8473
TOTAL                 3651.10 3651.10      0.  209958. 100.000
    
```

TOTAL LB 209958. 209958. 0.

STREAM NUMBER 1  
 TEMPERATURE DEG F 80.000  
 PRESSURE PSIA 210.00  
 ENTHALPY BTU/HR -2.71660E+07  
 VAPOR FRACTION 0.00000E+00

PROPERTIES	TOTAL	LIQUID
FLOWRATE LBMOL/HR	3651.1001	3651.1001
MOLECULAR WT.	57.5055	57.5055
ENTHALPY BTU/LBMOLE	-7440.4976	-7440.4976
ENTROPY BTU/LBMO/R	-13.7340	-13.7340
CP BTU/LBMOL/R		34.3776
CV BTU/LBMOL/R		27.2008
DENSITY LB/FT3		35.1420
Z-FACTOR		0.059344
FLOWRATE GAL/MIN T-P		744.9296
S.G. (TS/60) GPA STP		0.578848
VISCOSITY CP		0.153460
TH.COND BTU/FT/HR/F		0.063455
SURFACE TENSION DYNE/CM		10.2549
TS IS STANDARD TEMPERATURE AT	60.00	DEG F

### Page 30 of Final Run Printout

Notice that the Index of Flowsheet Calculations also shows the page number where the equipment calculations occurred.

PAGE	INDEX OF FLOWSHEET CALCULATIONS
1	ECHO PRINT OF INPUT DATA
6	++++ BEGIN ITERATION 1 OF RECYCLE LOOP 1 ++++
6	SHO 3 (DEC )
6	HEAEXC 1 (OVHD)
6	HEAEXC 2 (BOTS)
7	++++ BEGIN ITERATION 2 OF RECYCLE LOOP 1 ++++
7	SHO 3 (DEC )
10	HEAEXC 1 (OVHD)
10	HEAEXC 2 (BOTS)
11	++++ BEGIN ITERATION 3 OF RECYCLE LOOP 1 ++++
11	SHO 3 (DEC )
14	HEAEXC 1 (OVHD)
14	HEAEXC 2 (BOTS)
15	+++LOOP 1 HAS CONVERGED AFTER 3 ITERATIONS +++
16	SOLUTION REACHED
17	STREAM SUMMARY
20	EQUIPMENT SUMMARY - EXCHANGER/CONDENSERS
21	EQUIPMENT SUMMARY - SHORTCUT DISTILLATON
22	MATERIAL BALANCE SUMMARY
23	DETAILED PRINT FOR STREAM 1
24	DETAILED PRINT FOR STREAM 2
25	DETAILED PRINT FOR STREAM 3
26	DETAILED PRINT FOR STREAM 4
27	DETAILED PRINT FOR STREAM 5
28	DETAILED PRINT FOR STREAM 6
29	DETAILED PRINT FOR STREAM 7
30	INDEX OF FLOWSHEET CALCULATIONS
31	ACCOUNTING INFORMATION
30	ACCOUNTING INFORMATION

## Example Flowsheet Simulation-Debutanizer Column Design

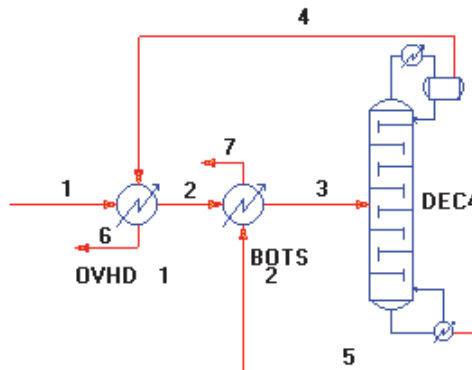
The objective of this simulation is to design and optimize a debutanizer column to maximize reboiler fuel savings. The column feed is from storage and is at 80°F. It is to be heated with the column overhead and then the bottoms in order to reduce reboiler requirements. (The coding for a rigorous, tray-by-tray calculation of the debutanizer is presented in DESIGN II Example Problems *Debutanizer Design Example*) The feed and operating conditions are as follows:

Feed	Component	Flow, LBMOL/HR
	C3	2000
	i-C4	400
	n-C4	600
	i-C5	150.3
	n-C5	200
	C6	50.8
	C7+	250

(API gravity = 40, mean average boiling point = 350, molecular weight = 136)

The total first-run input for this problem looks like this:

```
Account Number      AB123.
Title Command       *DEBUTANIZER DESIGN
Equipment           HEA EXC 1 = OVHD, 4, 1, -6, -2,
                   TEM APP= 10
Module              HEA EXC 2 = BOTS, 5,2, -7, -3, TEM APP= 20
Commands            SHO 3 = DEC4, 3, -4, -5, PRE TOP = 200
                   REC TOP 6 = .98, REC BOT 7 = .95, PAR
                   GEN,
                   COM = 4, 5, 6, 7, 8, 10, 100
                   API 100 = 40, AMB 100 = 350, AMW100 = 136
General             NAM 100 = C7+, MAX = 10
Commands            TP 1 = 80, 210
                   FLO 1 = 2000, 400, 600, 150.3, 200,50.8,250
END Command        END
```



## DESIGN II Limitations

DESIGN II basically has very few limitations. There is a maximum of 9,999 equipment modules and 9,999 streams per simulation. The number of components is limited to 1,000 per simulation. The number of Petroleum Fractions is limited to 600 per simulation. Any other limitations are equipment module or thermodynamic methods based and are documented at that location.



# Chapter 2: Database Components

## Component Database Sorted By ID

The DESIGN II Component Database contains 1235+ chemicals that are used in the Chemical Processing Industries. DESIGN II has assigned an internal ID number referring to each component. The following contain the various components according to DESIGN II ID numbers. **NOTE:** Some ID numbers are duplicated to represent the same component (formula) with different known names in literature.

The Mixed Amine column designates whether or not the chemical can be used with the Mixed Amine thermodynamics method in DESIGN II.

## Component Database - ID From 1 to 99

The components ID numbers between 1-99 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, heat capacity, critical temperature, critical pressure, acentric factor ( $w$ ) or critical volume  $V_c$ , solubility parameter ( $d$ ), and Molecular Weight.

DESIGN II ID	Name	Mixed Amine	Formula	Molecular Weight	BP (F)	BP (C)	BP (R)	BP (K)
1	HYDROGEN	Yes	H2	2.02	-423.00	-252.78	36.67	20.37
2	METHANE	Yes	CH4	16.04	-258.70	-161.50	200.97	111.65
3	ETHANE	Yes	C2H6	30.07	-127.48	-88.60	332.19	184.55
4	PROPANE	Yes	C3H8	44.09	-43.78	-42.10	415.89	231.05
4	REFRIGERANT 290	Yes	C3H8	44.09	-43.78	-42.10	415.89	231.05
4	R290	Yes	C3H8	44.09	-43.78	-42.10	415.89	231.05
4	R-290	Yes	C3H8	44.09	-43.78	-42.10	415.89	231.05
5	I-BUTANE	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
5	ISOBUTANE	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
5	REFRIGERANT 600A	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
5	R600A	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
5	2-METHYLPROPANE	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
5	R-600A	Yes	C4H10	58.12	10.71	-11.83	470.38	261.32
6	BUTANE	Yes	C4H10	58.12	31.14	-0.48	490.81	272.67
6	N-BUTANE	Yes	C4H10	58.12	31.14	-0.48	490.81	272.67
6	REFRIGERANT 600	Yes	C4H10	58.12	31.14	-0.48	490.81	272.67
6	R600	Yes	C4H10	58.12	31.14	-0.48	490.81	272.67
6	R-600	Yes	C4H10	58.12	31.14	-0.48	490.81	272.67
7	I-PENTANE	Yes	C5H12	72.15	83.98	28.88	543.65	302.03
7	ISOPENTANE	Yes	C5H12	72.15	83.98	28.88	543.65	302.03
7	2-METHYLBUTANE	Yes	C5H12	72.15	83.98	28.88	543.65	302.03
8	N-PENTANE	Yes	C5H12	72.15	96.88	36.04	556.55	309.19
9	2,2-DIMETHYLPROPANE	Yes	C5H12	72.15	49.06	9.48	508.73	282.63
9	NEO-PENTANE	Yes	C5H12	72.15	49.06	9.48	508.73	282.63
9	TERT-PENTANE	Yes	C5H12	72.15	49.06	9.48	508.73	282.63
10	N-HEXANE	Yes	C6H14	86.17	155.74	68.74	615.41	341.89
11	N-HEPTANE	Yes	C7H16	100.20	209.17	98.43	668.84	371.58
12	N-OCTANE	Yes	C8H18	114.22	258.22	125.68	717.89	398.83
13	N-NONANE	No	C9H20	128.25	303.48	150.82	763.15	423.97
14	N-DECANE	No	C10H22	142.28	345.47	174.15	805.14	447.30
15	N-UNDECANE	No	C11H24	156.30	384.67	195.93	844.34	469.08
16	N-DODECANE	No	C12H26	170.33	421.38	216.32	881.05	489.47
17	N-TRIDECANE	No	C13H28	184.35	455.84	235.47	915.51	508.62
18	N-TETRADECANE	No	C14H30	198.38	488.44	253.58	948.11	526.73
19	N-PENTADECANE	No	C15H32	212.41	519.23	270.68	978.90	543.83
20	N-HEXADECANE	No	C16H34	226.43	548.36	286.87	1008.03	560.02
21	N-HEPTADECANE	No	C17H36	240.46	575.64	302.02	1035.31	575.17
22	ETHENE	Yes	C2H4	28.05	-154.68	-103.71	304.99	169.44
22	ETHYLENE	Yes	C2H4	28.05	-154.68	-103.71	304.99	169.44
23	1-PROPENE	Yes	C3H6	42.08	-53.86	-47.70	405.81	225.45
23	PROPENE	Yes	C3H6	42.08	-53.86	-47.70	405.81	225.45
23	PROPYLENE	Yes	C3H6	42.08	-53.86	-47.70	405.81	225.45
24	1-BUTENE	Yes	C4H8	56.10	20.73	-6.26	480.40	266.89
25	CIS-2-BUTENE	No	C4H8	56.10	38.70	3.72	498.37	276.87
26	TRANS-2-BUTENE	No	C4H8	56.10	33.58	0.88	493.25	274.03
27	I-BUTENE	Yes	C4H8	56.10	19.58	-6.90	479.25	266.25
27	ISOBUTYLENE	Yes	C4H8	56.10	19.58	-6.90	479.25	266.25

## Chapter 2

27	ISOBUTENE	Yes	C4H8	56.10	19.58	-6.90	479.25	266.25
27	2-METHYL PROPENE	Yes	C4H8	56.10	19.58	-6.90	479.25	266.25
28	BIVINYL	Yes	C4H6	54.09	24.06	-4.41	483.73	268.74
28	1,3-BUTADIENE	Yes	C4H6	54.09	24.06	-4.41	483.73	268.74
29	1-PENTENE	No	C5H10	70.13	85.94	29.97	545.61	303.12
30	CIS-2-PENTENE	No	C5H10	70.13	98.50	36.94	558.17	310.09
31	TRANS-2-PENTENE	No	C5H10	70.13	97.44	36.36	557.11	309.51
32	2-METHYL-1-BUTENE	No	C5H10	70.13	88.09	31.16	547.76	304.31
33	3-METHYL-1-BUTENE	No	C5H10	70.13	68.11	20.06	527.78	293.21
34	2-METHYL-2-BUTENE	No	C5H10	70.13	101.42	38.57	561.09	311.72
35	1-HEXENE	No	C6H12	84.16	146.27	63.48	605.94	336.63
36	CYCLOPENTANE	Yes	C5H10	70.13	120.67	49.26	580.34	322.41
37	METHYLCYCLOPENTANE	Yes	C6H12	84.16	161.26	71.81	620.93	344.96
38	CYCLOHEXANE	Yes	C6H12	84.16	177.32	80.73	636.99	353.88
39	METHYLCYCLOHEXANE	Yes	C7H14	98.18	213.68	100.93	673.35	374.08
40	BENZENE	Yes	C6H6	78.11	176.18	80.10	635.85	353.25
40	BENZOL	Yes	C6H6	78.11	176.18	80.10	635.85	353.25
41	METHYL BENZENE	Yes	C7H8	92.13	231.13	110.63	690.80	383.78
41	PHENYL METHANE	Yes	C7H8	92.13	231.13	110.63	690.80	383.78
41	TOLUENE	Yes	C7H8	92.13	231.13	110.63	690.80	383.78
41	TOLUOL	Yes	C7H8	92.13	231.13	110.63	690.80	383.78
42	1,2-DIMETHYLBENZENE	Yes	C8H10	106.16	291.94	144.41	751.61	417.56
42	O-XYLENE	Yes	C8H10	106.16	291.94	144.41	751.61	417.56
42	O-XYLOL	Yes	C8H10	106.16	291.94	144.41	751.61	417.56
43	1,3-DIMETHYLBENZENE	Yes	C8H10	106.16	282.39	139.11	742.06	412.26
43	M-XYLENE	Yes	C8H10	106.16	282.39	139.11	742.06	412.26
43	M-XYLOL	Yes	C8H10	106.16	282.39	139.11	742.06	412.26
44	1,4-DIMETHYLBENZENE	Yes	C8H10	106.16	281.03	138.35	740.70	411.50
44	P-XYLENE	Yes	C8H10	106.16	281.03	138.35	740.70	411.50
44	P-XYLOL	Yes	C8H10	106.16	281.03	138.35	740.70	411.50
45	ETHYL BENZENE	Yes	C8H10	106.16	277.14	136.19	736.81	409.34
46	NITROGEN	Yes	N2	28.01	-320.40	-195.78	139.27	77.37
47	OXYGEN	Yes	O2	32.00	-297.40	-183.00	162.27	90.15
48	CARBON MONOXIDE	Yes	CO	28.01	-313.60	-192.00	146.07	81.15
49	CARBON DIOXIDE	Yes	CO2	44.01	-109.30	-78.50	350.37	194.65
49	REFRIGERANT 744	Yes	CO2	44.01	-109.30	-78.50	350.37	194.65
49	R744	Yes	CO2	44.01	-109.30	-78.50	350.37	194.65
49	R-744	Yes	CO2	44.01	-109.30	-78.50	350.37	194.65
50	HYDROGEN SULFIDE	Yes	H2S	34.08	-76.60	-60.33	383.07	212.82
51	SULFUR DIOXIDE	No	SO2	64.06	14.00	-10.00	473.67	263.15
52	2-METHYLPENTANE	No	C6H14	86.20	140.49	60.27	600.16	333.42
53	3-METHYLPENTANE	No	C6H14	86.20	145.91	63.28	605.58	336.43
54	2,2-DIMETHYLBUTANE	No	C6H14	86.20	121.53	49.74	581.20	322.89
54	NEOHEXANE	No	C6H14	86.20	121.53	49.74	581.20	322.89
55	2,3-DIMETHYLBUTANE	No	C6H14	86.20	136.38	57.99	596.05	331.14
56	1-HEPTENE	No	C7H14	98.20	200.56	93.64	660.23	366.79
57	ALLENE	No	C3H4	40.10	-29.90	-34.39	429.77	238.76
57	PROPADIENE	No	C3H4	40.10	-29.90	-34.39	429.77	238.76
58	1,2-BUTADIENE	No	C4H6	54.10	51.53	10.85	511.20	284.00
58	METHYL ALLENE	No	C4H6	54.10	51.53	10.85	511.20	284.00
59	ETHYLCYCLOPENTANE	No	C7H14	98.20	218.24	103.47	677.91	376.62
60	ETHYLCYCLOHEXANE	No	C8H16	112.20	269.23	131.79	728.90	404.94
61	ISOPRENE	No	C5H8	68.10	93.31	34.06	552.98	307.21
61	2-METHYL-1,3-BUTADIENE	No	C5H8	68.10	93.31	34.06	552.98	307.21
62	WATER	Yes	H2O	18.02	212.00	100.00	671.67	373.15
63	AMMONIA	No	NH3	17.03	-28.20	-33.44	431.47	239.71
63	REFRIGERANT 717	No	NH3	17.03	-28.20	-33.44	431.47	239.71
63	R717	No	NH3	17.03	-28.20	-33.44	431.47	239.71
63	R-717	No	NH3	17.03	-28.20	-33.44	431.47	239.71
64	CARBON	No	C	12.01	7560.00	4182.22	8019.67	4455.37
65	ACETYLENE	Yes	C2H2	26.04	-119.20	-84.00	340.47	189.15
65	ETHYNE	Yes	C2H2	26.04	-119.20	-84.00	340.47	189.15
66	METHYLACETYLENE	Yes	C3H4	40.06	-9.78	-23.21	449.89	249.94
66	PROPYNE	Yes	C3H4	40.06	-9.78	-23.21	449.89	249.94
67	1-BUTYNE	Yes	C4H6	54.09	46.54	8.08	506.21	281.23
67	ETHYLACETYLENE	Yes	C4H6	54.09	46.54	8.08	506.21	281.23
68	2-METHYLPROPENE	No	C4H8	56.10	19.58	-6.90	479.25	266.25
69	CYCLOPENTENE	No	C5H8	68.11	111.62	44.23	571.29	317.38
70	N-PROPYLBENZENE	No	C9H12	120.19	318.59	159.22	778.26	432.37
71	ISOPROPYLBENZENE	No	C9H12	120.19	306.31	152.39	765.98	425.54
71	CUMENE	No	C9H12	120.19	306.31	152.39	765.98	425.54

72	O-ETHYLTOLUENE	No	C9H12	120.19	329.28	165.16	788.95	438.31
72	1-METHYL-2-ETHYLBENZENE	No	C9H12	120.19	329.28	165.16	788.95	438.31
73	M-ETHYLTOLUENE	No	C9H12	120.19	322.35	161.31	782.02	434.46
73	1-METHYL-3-ETHYLBENZENE	No	C9H12	120.19	322.35	161.31	782.02	434.46
74	P-ETHYLTOLUENE	No	C9H12	120.19	323.58	161.99	783.25	435.14
74	1-METHYL-4-ETHYLBENZENE	No	C9H12	120.19	323.58	161.99	783.25	435.14
75	HEMIMELLITENE	No	C9H12	120.19	348.95	176.08	808.62	449.23
75	1,2,3-MESITYLENE	No	C9H12	120.19	348.95	176.08	808.62	449.23
75	1,2,3-TRIMETHYLBENZENE	No	C9H12	120.19	348.95	176.08	808.62	449.23
76	1,2,4-MESITYLENE	No	C9H12	120.19	336.83	169.35	796.50	442.50
76	PSEUDOCUMENE	No	C9H12	120.19	336.83	169.35	796.50	442.50
76	1,2,4-TRIMETHYLBENZENE	No	C9H12	120.19	336.83	169.35	796.50	442.50
77	1,3,5-MESITYLENE	No	C9H12	120.19	328.49	164.72	788.16	437.87
77	1,3,5-TRIMETHYLBENZENE	No	C9H12	120.19	328.49	164.72	788.16	437.87
78	N-BUTYLBENZENE	No	C10H14	134.21	361.95	183.31	821.62	456.46
79	ISOHEPTANE	Yes	C7H16	100.20	194.09	90.05	653.76	363.20
79	2-METHYLHEXANE	Yes	C7H16	100.20	194.09	90.05	653.76	363.20
80	3-METHYLHEXANE	No	C7H16	100.20	197.33	91.85	657.00	365.00
81	2-METHYLHEPTANE	No	C8H18	114.22	243.77	117.65	703.44	390.80
82	ISOCTANE	No	C8H18	114.22	210.63	99.24	670.30	372.39
82	2,2,4-TRIMETHYLPENTANE	No	C8H18	114.22	210.63	99.24	670.30	372.39
83	1-OCTENE	No	C8H16	112.21	250.30	121.28	709.97	394.43
84	CYCLOPENTENE	No	C5H8	68.11	111.62	44.23	571.29	317.38
85	TRANS-1,3-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	256.02	124.46	715.69	397.61
86	CIS-1,4-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	255.79	124.33	715.46	397.48
87	TRANS-1,4-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	246.84	119.36	706.51	392.51
88	1,1-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	247.19	119.55	706.86	392.70
89	CIS-1,2-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	265.53	129.74	725.20	402.89
90	CIS-1,3-DIMETHYLCYCLOHEXANE	No	C8H16	112.21	248.17	120.09	707.84	393.24
91	N-OCTADECANE	No	C18H38	254.48	601.30	316.28	1060.97	589.43
92	N-NONADECANE	No	C19H40	268.51	625.80	329.89	1085.47	603.04
93	DIDECYL	No	C20H42	282.54	650.80	343.78	1110.47	616.93
93	N-EICOSANE	No	C20H42	282.54	650.80	343.78	1110.47	616.93
94	1,1-DIMETHYLCYCLOPENTANE	No	C7H14	98.18	190.12	87.84	649.79	360.99
95	CIS-1,2-DIMETHYLCYCLOPENTANE	No	C7H14	98.18	211.16	99.53	670.83	372.68
96	TRANS-1,2-DIMETHYLCYCLOPENTANE	No	C7H14	98.18	197.36	91.87	657.03	365.02
97	CIS-1,3-DIMETHYLCYCLOPENTANE	No	C7H14	98.18	195.39	90.77	655.06	363.92
98	TRANS-1,3-DIMETHYLCYCLOPENTANE	No	C7H14	98.18	197.11	91.73	656.78	364.88
99	AIR	No	AIR	28.96	-317.60	-194.22	142.07	78.93

## Component Database - ID From 100 to 999

The component ID numbers between 100 to 999 are used within DESIGN II when the user decides to provide component data according to the following categories.

100-199 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

200-299 User-provided nonstandard or special chemical component data. See ChemTran: Component Properties Command Details

300-399 User-provided solid component data. See ChemTran or ChemTran: Entering Data for Solid Components (300)

400-499 Reserved for future use

500-599 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

600-699 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

700-799 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

800-899 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

900-999 User-provided petroleum fraction data. See Petroleum (Pseudo) Fractions

## Component Database - ID From 1000 to 1999

The components ID numbers between 1000-1999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, heat capacity, critical temperature, critical pressure, and vapor pressure (as a function of temperature in range at least from 200 to 760 mmHg). For other properties see *Component Properties Estimation Methods*.

DESIGN II ID	Name	Mixed Amine	Formula	Molecular Weight	BP (F)	BP (C)	BP (R)	BP (K)
1000	HYDROGEN (PARA)	No	H2 (para)	2.02	-423.00	-252.78	36.67	20.37
1001	ACETIC ACID	No	C2H4O2	60.05	244.22	117.90	703.89	391.05
1001	ETHANOIC ACID	No	C2H4O2	60.05	244.22	117.90	703.89	391.05
1002	ACETONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44
1002	DIMETHYL KETONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44

## Chapter 2

1000	HYDROGEN(PARA)	No	H2	2.02	-423.00	-252.78	36.67	20.37
1001	ACETIC ACID	No	C2H4O2	60.05	244.22	117.90	703.89	391.05
1001	ETHANOIC ACID	No	C2H4O2	60.05	244.22	117.90	703.89	391.05
1002	ACETONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44
1002	DIMETHYL KETONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44
1002	METHYL KETONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44
1002	2-PROPANONE	No	C3H6O	58.08	133.32	56.29	592.99	329.44
1003	ACETONITRILE	No	C2H3N	41.05	178.97	81.65	638.64	354.80
1003	CYANOMETHANE	No	C2H3N	41.05	178.97	81.65	638.64	354.80
1003	ETHANENITRILE	No	C2H3N	41.05	178.97	81.65	638.64	354.80
1003	METHYL CYANIDE	No	C2H3N	41.05	178.97	81.65	638.64	354.80
1004	AMINO BENZENE	No	C6H7N	93.12	363.92	184.40	823.59	457.55
1004	ANILINE	No	C6H7N	93.12	363.92	184.40	823.59	457.55
1004	PHENYLAMINE	No	C6H7N	93.12	363.92	184.40	823.59	457.55
1005	DIETHYL ETHER	No	C4H10O	74.12	94.19	34.55	553.86	307.70
1005	ETHOXYETHANE	No	C4H10O	74.12	94.19	34.55	553.86	307.70
1005	ETHYL ETHER	No	C4H10O	74.12	94.19	34.55	553.86	307.70
1005	ETHER	No	C4H10O	74.12	94.19	34.55	553.86	307.70
1006	BROMOBENZENE	No	C6H5BR	157.02	313.07	156.15	772.74	429.30
1006	PHENYL BROMIDE	No	C6H5BR	157.02	313.07	156.15	772.74	429.30
1007	CHLOROBENZENE	No	C6H5CL	112.56	269.06	131.70	728.73	404.85
1007	PHENYL CHLORIDE	No	C6H5CL	112.56	269.06	131.70	728.73	404.85
1008	CHLOROFORM	No	CHCL3	119.39	143.11	61.73	602.78	334.88
1008	TRICHLOROMETHANE	No	CHCL3	119.39	143.11	61.73	602.78	334.88
1010	DIMETHYL ETHER	No	C2H6O	46.07	-12.71	-24.84	446.96	248.31
1010	METHYL ETHER	No	C2H6O	46.07	-12.71	-24.84	446.96	248.31
1011	DIMETHYL SULFIDE	No	C2H6S	62.13	99.20	37.33	558.87	310.48
1011	METHYL SULFIDE	No	C2H6S	62.13	99.20	37.33	558.87	310.48
1012	ETHANOL	No	C2H6O	46.07	172.92	78.29	632.59	351.44
1012	ETHYL ALCOHOL	No	C2H6O	46.07	172.92	78.29	632.59	351.44
1012	METHYL CARBINOL	No	C2H6O	46.07	172.92	78.29	632.59	351.44
1013	EPOXYETHANE	No	C2H4O	44.05	51.01	10.56	510.68	283.71
1013	ETHYLENE OXIDE	No	C2H4O	44.05	51.01	10.56	510.68	283.71
1013	OXIRANE	No	C2H4O	44.05	51.01	10.56	510.68	283.71
1014	AMINOETHANE	No	C2H7N	45.08	61.84	16.58	521.51	289.73
1014	ETHYLAMINE	No	C2H7N	45.08	61.84	16.58	521.51	289.73
1015	CHLOROETHANE	No	C2H5CL	64.52	54.09	12.27	513.76	285.42
1015	ETHYL CHLORIDE	No	C2H5CL	64.52	54.09	12.27	513.76	285.42
1016	ETHANETHIOL	No	C2H6S	62.13	95.00	35.00	554.67	308.15
1016	ETHYL HYDROSULFIDE	No	C2H6S	62.13	95.00	35.00	554.67	308.15
1016	ETHYL MERCAPTAN	No	C2H6S	62.13	95.00	35.00	554.67	308.15
1016	ETHYL THIOALCOHOL	No	C2H6S	62.13	95.00	35.00	554.67	308.15
1017	HYDROCHLORIC ACID	No	HCL	36.47	-121.06	-85.03	338.61	188.12
1017	HYDROGEN CHLORIDE	No	HCL	36.47	-121.06	-85.03	338.61	188.12
1018	HYDROGEN CYANIDE	No	HCN	27.03	78.26	25.70	537.93	298.85
1019	ISOPROPANOL	No	C3H8O	60.09	180.07	82.26	639.74	355.41
1019	ISOPROPYL ALCOHOL	No	C3H8O	60.09	180.07	82.26	639.74	355.41
1019	2-PROPANOL	No	C3H8O	60.09	180.07	82.26	639.74	355.41
1020	2-BUTANONE	No	C4H8O	72.10	175.35	79.64	635.02	352.79
1020	ETHYL METHYL KETONE	No	C4H8O	72.10	175.35	79.64	635.02	352.79
1020	METHYL ETHYL KETONE	No	C4H8O	72.10	175.35	79.64	635.02	352.79
1021	METHANOL	No	CH4O	32.04	148.46	64.70	608.13	337.85
1021	METHYL ALCOHOL	No	CH4O	32.04	148.46	64.70	608.13	337.85
1022	1-BUTANOL	No	C4H10O	74.12	243.79	117.66	703.46	390.81
1022	N-BUTANOL	No	C4H10O	74.12	243.79	117.66	703.46	390.81
1022	BUTANOL	No	C4H10O	74.12	243.79	117.66	703.46	390.81
1022	N-BUTYL ALCOHOL	No	C4H10O	74.12	243.79	117.66	703.46	390.81
1023	1-PROPANOL	No	C3H8O	60.09	206.96	97.20	666.63	370.35
1023	N-PROPANOL	No	C3H8O	60.09	206.96	97.20	666.63	370.35
1023	N-PROPYL ALCOHOL	No	C3H8O	60.09	206.96	97.20	666.63	370.35
1024	THIOFURAN	No	C4H4S	84.14	183.49	84.16	643.16	357.31
1024	THIOPHENE	No	C4H4S	84.14	183.49	84.16	643.16	357.31
1025	2-BUTANOL	No	C4H10O	74.12	211.19	99.55	670.86	372.70
1025	SEC-BUTYL ALCOHOL	No	C4H10O	74.12	211.19	99.55	670.86	372.70
1026	T-BUTYL ALCOHOL	No	C4H10O	74.12	180.36	82.42	640.03	355.57
1026	2-METHYL-2-PROPANOL	No	C4H10O	74.12	180.36	82.42	640.03	355.57
1027	CARBON TETRACHLORIDE	No	CCL4	153.84	170.15	76.75	629.82	349.90
1027	TETRACHLOROMETHANE	No	CCL4	153.84	170.15	76.75	629.82	349.90
1027	REFRIGERANT 10	No	CCL4	153.84	170.15	76.75	629.82	349.90
1027	R10	No	CCL4	153.84	170.15	76.75	629.82	349.90
1027	FREON 10	No	CCL4	153.84	170.15	76.75	629.82	349.90

# Database Components

1027	R-10	No	CCL4	153.84	170.15	76.75	629.82	349.90
1028	1,2-DICHLOROETHANE	No	C2H4CL2	98.97	182.25	83.47	641.92	356.62
1028	ETHYLENE DICHLORIDE	No	C2H4CL2	98.97	182.25	83.47	641.92	356.62
1029	DIETHYLAMINE	No	C4H11N	73.14	129.47	54.15	589.14	327.30
1030	DIETHYLENE DIOXIDE	No	C4H8O2	88.10	214.07	101.15	673.74	374.30
1030	DIOXANE	No	C4H8O2	88.10	214.07	101.15	673.74	374.30
1030	1,4-DIOXANE	No	C4H8O2	88.10	214.07	101.15	673.74	374.30
1030	P-DIOXANE	No	C4H8O2	88.10	214.07	101.15	673.74	374.30
1031	ETHYL ACETATE	No	C4H8O2	88.10	168.80	76.00	628.47	349.15
1032	BROMOETHANE	No	C2H5BR	108.98	101.03	38.35	560.70	311.50
1032	ETHYL BROMIDE	No	C2H5BR	108.98	101.03	38.35	560.70	311.50
1033	DIETHYL SULFIDE	No	C4H10S	90.19	197.78	92.10	657.45	365.25
1033	ETHYL SULFIDE	No	C4H10S	90.19	197.78	92.10	657.45	365.25
1033	3-THIOPENTANE	No	C4H10S	90.19	197.78	92.10	657.45	365.25
1034	FLUOROBENZENE	No	C6H5F	96.10	184.53	84.74	644.20	357.89
1034	PHENYL FLUORIDE	No	C6H5F	96.10	184.53	84.74	644.20	357.89
1035	IODOBENZENE	No	C6H5I	204.01	370.99	188.33	830.66	461.48
1035	PHENYL IODIDE	No	C6H5I	204.01	370.99	188.33	830.66	461.48
1036	3-CRESOL	No	C7H8O	108.13	396.02	202.23	855.69	475.38
1036	M-CRESOL	No	C7H8O	108.13	396.02	202.23	855.69	475.38
1036	3-HYDROXY TOLUENE	No	C7H8O	108.13	396.02	202.23	855.69	475.38
1036	3-METHYLPHENOL	No	C7H8O	108.13	396.02	202.23	855.69	475.38
1037	CHLOROMETHANE	No	CH3CL	50.49	-11.60	-24.22	448.07	248.93
1037	METHYL CHLORIDE	No	CH3CL	50.49	-11.60	-24.22	448.07	248.93
1038	ETHYL METHYL ETHER	No	C3H8O	60.09	45.23	7.35	504.90	280.50
1038	METHYL ETHYL ETHER	No	C3H8O	60.09	45.23	7.35	504.90	280.50
1039	FLUOROMETHANE	No	CH3F	34.03	-109.03	-78.35	350.64	194.80
1039	METHYL FLUORIDE	No	CH3F	34.03	-109.03	-78.35	350.64	194.80
1040	METHYL FORMATE	No	C2H4O2	60.05	88.79	31.55	548.46	304.70
1041	NITRIC OXIDE	No	NO	30.09	-241.19	-151.77	218.48	121.38
1041	NITROGEN OXIDE	No	NO	30.09	-241.19	-151.77	218.48	121.38
1041	NITROGEN MONOXIDE	No	NO	30.09	-241.19	-151.77	218.48	121.38
1042	NITROMETHANE	No	CH3NO2	61.04	214.14	101.19	673.81	374.34
1043	DINITROGEN OXIDE	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1043	DINITROGEN MONOXIDE	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1043	REFRIGERANT 744A	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1043	R744A	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1043	R-744A	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1043	NITROUS OXIDE	No	N2O	44.01	-127.26	-88.48	332.41	184.67
1044	ETHYL CYANIDE	No	C3H5N	55.08	206.91	97.17	666.58	370.32
1044	PROPANENITRILE	No	C3H5N	55.08	206.91	97.17	666.58	370.32
1044	PROPIONITRILE	No	C3H5N	55.08	206.91	97.17	666.58	370.32
1045	AZINE	No	C5H5N	79.10	239.41	115.23	699.08	388.38
1045	PYRIDINE	No	C5H5N	79.10	239.41	115.23	699.08	388.38
1046	TRIETHYL AMINE	No	C6H15N	101.19	193.19	89.55	652.86	362.70
1047	TRIMETHYL AMINE	No	C3H9N	59.11	37.17	2.87	496.84	276.02
1048	1,2-EPOXY PROPANE	No	C3H6O	58.08	94.10	34.50	553.77	307.65
1048	METHYL OXIRANE	No	C3H6O	58.08	94.10	34.50	553.77	307.65
1048	PROPYLENE OXIDE	No	C3H6O	58.08	94.10	34.50	553.77	307.65
1049	METHYL N-PROPYL KETONE	No	C5H10O	86.13	216.16	102.31	675.83	375.46
1049	2-PENTANONE	No	C5H10O	86.13	216.16	102.31	675.83	375.46
1050	DIISOPROPYL ETHER	No	C6H14O	102.17	153.59	67.55	613.26	340.70
1050	ISOPROPYL ETHER	No	C6H14O	102.17	153.59	67.55	613.26	340.70
1051	1,4-EPOXY-1,3-BUTADIENE	No	C4H4O	68.07	88.43	31.35	548.10	304.50
1051	FURAN	No	C4H4O	68.07	88.43	31.35	548.10	304.50
1051	FURFURAN	No	C4H4O	68.07	88.43	31.35	548.10	304.50
1052	CARBON TETRAFLUORIDE	No	CF4	88.01	-197.86	-127.70	261.81	145.45
1052	TETRAFLUOROMETHANE	No	CF4	88.01	-197.86	-127.70	261.81	145.45
1052	REFRIGERANT 14	No	CF4	88.01	-197.86	-127.70	261.81	145.45
1052	R14	No	CF4	88.01	-197.86	-127.70	261.81	145.45
1052	R-14	No	CF4	88.01	-197.86	-127.70	261.81	145.45
1053	OCTAFLUOROCYCLOBUTANE	No	C4F8	200.04	21.24	-5.98	480.91	267.17
1053	PERFLUOROCYCLOBUTANE	No	C4F8	200.04	21.24	-5.98	480.91	267.17
1053	REFRIGERANT C318	No	C4F8	200.04	21.24	-5.98	480.91	267.17
1053	RC318	No	C4F8	200.04	21.24	-5.98	480.91	267.17
1053	RC-318	No	C4F8	200.04	21.24	-5.98	480.91	267.17
1055	1,1-DIFLUOROETHANE	No	C2H4F2	66.05	-12.46	-24.70	447.21	248.45
1055	REFRIGERANT 152A	No	C2H4F2	66.05	-12.46	-24.70	447.21	248.45
1055	FREON 152A	No	C2H4F2	66.05	-12.46	-24.70	447.21	248.45
1055	R152A	No	C2H4F2	66.05	-12.46	-24.70	447.21	248.45
1055	R-152A	No	C2H4F2	66.05	-12.46	-24.70	447.21	248.45

## Chapter 2

1056	1,1,1-TRIFLUOROETHANE	No	C2H3F3	84.04	-53.12	-47.29	406.55	225.86
1056	REFRIGERANT 143A	No	C2H3F3	84.04	-53.12	-47.29	406.55	225.86
1056	FREON 143A	No	C2H3F3	84.04	-53.12	-47.29	406.55	225.86
1056	R143A	No	C2H3F3	84.04	-53.12	-47.29	406.55	225.86
1056	R-143A	No	C2H3F3	84.04	-53.12	-47.29	406.55	225.86
1058	1,1-DICHLOROETHANE	No	C2H4CL2	98.97	135.10	57.28	594.77	330.43
1058	REFRIGERANT 150A	No	C2H4CL2	98.97	135.10	57.28	594.77	330.43
1058	FREON 150A	No	C2H4CL2	98.97	135.10	57.28	594.77	330.43
1058	R150A	No	C2H4CL2	98.97	135.10	57.28	594.77	330.43
1058	R-150A	No	C2H4CL2	98.97	135.10	57.28	594.77	330.43
1059	METHANETHIOL	No	CH4S	48.11	42.73	5.96	502.40	279.11
1059	METHYL MERCAPTAN	No	CH4S	48.11	42.73	5.96	502.40	279.11
1060	FLUORINE	No	F2	38.00	-306.63	-188.13	153.04	85.02
1061	1-AZACYCLOPENTENE	No	C4H9N	71.12	187.83	86.57	647.50	359.72
1061	PYRROLIDINE	No	C4H9N	71.12	187.83	86.57	647.50	359.72
1061	TETRAHYDROPYRROLE	No	C4H9N	71.12	187.83	86.57	647.50	359.72
1062	CHLORINE	No	CL2	70.91	-29.29	-34.05	430.38	239.10
1063	OZONE	No	O3	48.00	-168.34	-111.30	291.33	161.85
1064	CARBONIC ACID DICHLORIDE	No	COCL2	98.92	45.59	7.55	505.26	280.70
1064	CARBONYL CHLORIDE	No	COCL2	98.92	45.59	7.55	505.26	280.70
1064	CHLOROFORMYL CHLORIDE	No	COCL2	98.92	45.59	7.55	505.26	280.70
1064	PHOSGENE	No	COCL2	98.92	45.59	7.55	505.26	280.70
1065	FURAL	No	C5H4O2	96.08	323.06	161.70	782.73	434.85
1065	FURALDEHYDE	No	C5H4O2	96.08	323.06	161.70	782.73	434.85
1065	2-FURANCARBOXALDEHYDE	No	C5H4O2	96.08	323.06	161.70	782.73	434.85
1065	FURFURAL	No	C5H4O2	96.08	323.06	161.70	782.73	434.85
1065	FURFURALDEHYDE	No	C5H4O2	96.08	323.06	161.70	782.73	434.85
1067	SULFUR DIOXIDE	No	SO2	64.07	13.97	-10.02	473.64	263.13
1068	SULFUR TRIOXIDE	No	SO3	80.07	112.55	44.75	572.22	317.90
1069	CARBON DISULFIDE	No	CS2	76.14	115.70	46.50	575.37	319.65
1070	ACETIC ANHYDRIDE	No	C4H6O3	102.09	281.57	138.65	741.24	411.80
1070	ETHANOIC ANHYDRIDE	No	C4H6O3	102.09	281.57	138.65	741.24	411.80
1071	CYCLOHEXANOL	No	C6H12O	100.16	321.53	160.85	781.20	434.00
1071	HEXAHYDROPHENOL	No	C6H12O	100.16	321.53	160.85	781.20	434.00
1071	HEXALIN	No	C6H12O	100.16	321.53	160.85	781.20	434.00
1072	CYCLOHEXANONE	No	C6H10O	98.14	312.17	155.65	771.84	428.80
1072	KETOHEXAMETHYLENE	No	C6H10O	98.14	312.17	155.65	771.84	428.80
1072	PIMELIC KETONE	No	C6H10O	98.14	312.17	155.65	771.84	428.80
1074	ETHYL FLUORIDE	No	C2H5F	48.06	-35.77	-37.65	423.90	235.50
1074	FLUOROETHANE	No	C2H5F	48.06	-35.77	-37.65	423.90	235.50
1075	DICHLOROMETHANE	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1075	METHYLENE CHLORIDE	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1075	REFRIGERANT 30	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1075	R30	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1075	FREON 30	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1075	R-30	No	CH2CL2	84.94	103.55	39.75	563.22	312.90
1076	1-CHLOROPROPANE	No	C3H7CL	78.54	115.88	46.60	575.55	319.75
1076	N-PROPYL CHLORIDE	No	C3H7CL	78.54	115.88	46.60	575.55	319.75
1077	AMINOMETHANE	No	CH5N	31.06	20.39	-6.45	480.06	266.70
1077	METHYL AMINE	No	CH5N	31.06	20.39	-6.45	480.06	266.70
1077	REFRIGERANT 630	No	CH5N	31.06	20.39	-6.45	480.06	266.70
1077	R630	No	CH5N	31.06	20.39	-6.45	480.06	266.70
1077	R-630	No	CH5N	31.06	20.39	-6.45	480.06	266.70
1079	1-AMINOPROPANE	No	C3H9N	59.11	118.04	47.80	577.71	320.95
1079	N-PROPYLAMINE	No	C3H9N	59.11	118.04	47.80	577.71	320.95
1080	1-AMINOBUTANE	No	C4H11N	73.14	172.04	77.80	631.71	350.95
1080	N-BUTYLAMINE	No	C4H11N	73.14	172.04	77.80	631.71	350.95
1081	DIMETHYLAMINE	No	C2H7N	45.08	44.40	6.89	504.07	280.04
1082	BUTANENITRILE	No	C4H7N	69.10	243.18	117.32	702.85	390.47
1082	BUTYRONITRILE	No	C4H7N	69.10	243.18	117.32	702.85	390.47
1082	PROPYL CYANIDE	No	C4H7N	69.10	243.18	117.32	702.85	390.47
1083	BENZONITRILE	No	C7H5N	103.12	375.80	191.00	835.47	464.15
1084	PERCHLORYL FLUORIDE	No	CLO3F	102.46	-52.04	-46.69	407.63	226.46
1085	HYDROBROMIC ACID	No	HBR	80.92	-88.10	-66.72	371.57	206.43
1085	HYDROGEN BROMIDE	No	HBR	80.92	-88.10	-66.72	371.57	206.43
1086	HYDROGEN IODIDE	No	HI	127.92	-32.08	-35.60	427.59	237.55
1086	HYDROIODIC ACID	No	HI	127.92	-32.08	-35.60	427.59	237.55
1087	CARBON OXY SULFIDE	Yes	COS	60.08	-58.41	-50.23	401.26	222.92
1087	CARBONYL SULFIDE	Yes	COS	60.08	-58.41	-50.23	401.26	222.92
1088	BENZENOL	No	C6H6O	94.11	359.31	181.84	818.98	454.99
1088	CARBOLIC ACID	No	C6H6O	94.11	359.31	181.84	818.98	454.99

# Database Components

1088	HYDROXY BENZENE	No	C6H6O	94.11	359.31	181.84	818.98	454.99
1088	PHENOL	No	C6H6O	94.11	359.31	181.84	818.98	454.99
1089	2-CRESOL	No	C7H8O	108.13	375.81	191.01	835.48	464.16
1089	O-CRESOL	No	C7H8O	108.13	375.81	191.01	835.48	464.16
1089	2-HYDROXYTOLUENE	No	C7H8O	108.13	375.81	191.01	835.48	464.16
1089	2-METHYLPHENOL	No	C7H8O	108.13	375.81	191.01	835.48	464.16
1090	4-CRESOL	No	C7H8O	108.13	395.49	201.94	855.16	475.09
1090	P-CRESOL	No	C7H8O	108.13	395.49	201.94	855.16	475.09
1090	4-HYDROXYTOLUENE	No	C7H8O	108.13	395.49	201.94	855.16	475.09
1090	4-METHYLPHENOL	No	C7H8O	108.13	395.49	201.94	855.16	475.09
1099	DICHLOROFLUOROMETHANE	No	CHFCL2	102.92	48.02	8.90	507.69	282.05
1099	REFRIGERANT 21	No	CHFCL2	102.92	48.02	8.90	507.69	282.05
1099	R21	No	CHFCL2	102.92	48.02	8.90	507.69	282.05
1099	R-21	No	CHFCL2	102.92	48.02	8.90	507.69	282.05
1101	NITROGEN TRIFLUORIDE	No	NF3	71.00	-200.31	-129.06	259.36	144.09
1103	BORON TRIFLUORIDE	No	BF3	67.82	-149.26	-100.70	310.41	172.45
1104	BORON TRICHLORIDE	No	BCL3	117.19	54.86	12.70	514.53	285.85
1107	PHOSPHENE	No	PH3	34.00	-125.50	-87.50	334.17	185.65
1107	PHOSPHINE	No	PH3	34.00	-125.50	-87.50	334.17	185.65
1107	PHOSPHOROUS HYDRIDE	No	PH3	34.00	-125.50	-87.50	334.17	185.65
1107	PHOSPHOROUS TRIHYDRIDE	No	PH3	34.00	-125.50	-87.50	334.17	185.65
1108	SILANE	No	SIH4	32.09	-168.70	-111.50	290.97	161.65
1108	SILICANE	No	SIH4	32.09	-168.70	-111.50	290.97	161.65
1109	TETRAFLUROETHYLENE	No	C2F4	100.02	-104.12	-75.62	355.55	197.53
1109	REFRIGERANT 1114	No	C2F4	100.02	-104.12	-75.62	355.55	197.53
1109	R1114	No	C2F4	100.02	-104.12	-75.62	355.55	197.53
1109	R-1114	No	C2F4	100.02	-104.12	-75.62	355.55	197.53
1110	1,1-DIFLUOROETHENE	No	C2H2F2	64.04	-122.17	-85.65	337.50	187.50
1110	1,1-DIFLUOROETHYLENE	No	C2H2F2	64.04	-122.17	-85.65	337.50	187.50
1110	GENETRON 1132A	No	C2H2F2	64.04	-122.17	-85.65	337.50	187.50
1111	DIBROMOMETHANE	No	CBR2H2	173.84	209.57	98.65	669.24	371.80
1111	METHYLENE DIBROMIDE	No	CBR2H2	173.84	209.57	98.65	669.24	371.80
1112	HYDROGEN SELENIDE	No	SEH2	81.22	-42.43	-41.35	417.24	231.80
1112	SELENIUM HYDRIDE	No	SEH2	81.22	-42.43	-41.35	417.24	231.80
1113	HYDROGEN FLUORIDE	No	HF	20.01	67.91	19.95	527.58	293.10
1114	FLUROFORM	No	CHF3	70.02	-115.92	-82.18	343.75	190.97
1114	TRIFLUOROMETHANE	No	CHF3	70.02	-115.92	-82.18	343.75	190.97
1114	REFRIGERANT 23	No	CHF3	70.02	-115.92	-82.18	343.75	190.97
1114	R23	No	CHF3	70.02	-115.92	-82.18	343.75	190.97
1114	R-23	No	CHF3	70.02	-115.92	-82.18	343.75	190.97
1115	1,2-DIBROMOETHANE	No	C2H4BR2	187.88	268.97	131.65	728.64	404.80
1115	ETHYLENE DIBROMIDE	No	C2H4BR2	187.88	268.97	131.65	728.64	404.80
1116	BROMOTRIFLUOROMETHANE	No	CF3BR	148.91	-71.63	-57.57	388.04	215.58
1116	REFRIGERANT 13B1	No	CF3BR	148.91	-71.63	-57.57	388.04	215.58
1116	FREON 13B1	No	CF3BR	148.91	-71.63	-57.57	388.04	215.58
1116	R13B1	No	CF3BR	148.91	-71.63	-57.57	388.04	215.58
1116	R-13B1	No	CF3BR	148.91	-71.63	-57.57	388.04	215.58
1117	STANNIC CHLORIDE	No	SNCL4	260.53	237.38	114.10	697.05	387.25
1118	HEXAFLUROETHANE	No	C2F6	138.02	-108.90	-78.28	350.77	194.87
1118	PERFLUROETHANE	No	C2F6	138.02	-108.90	-78.28	350.77	194.87
1119	NITROSYL CHLORIDE	No	CLNO	65.46	22.32	-5.38	481.99	267.77
1120	HYDRAZINE	No	H4N2	32.05	236.30	113.50	695.97	386.65
1121	1,1,1-TRIFLUOROETHANE	No	C2F3H3	84.04	-53.68	-47.60	405.99	225.55
1121	REFRIGERANT 143A	No	C2F3H3	84.04	-53.68	-47.60	405.99	225.55
1121	R143A	No	C2F3H3	84.04	-53.68	-47.60	405.99	225.55
1121	R-143A	No	C2F3H3	84.04	-53.68	-47.60	405.99	225.55
1122	CHLOROPENTAFLUROETHANE	No	C2CLF5	154.47	-36.67	-38.15	423.00	235.00
1122	REFRIGERANT 115	No	C2CLF5	154.47	-36.67	-38.15	423.00	235.00
1122	R115	No	C2CLF5	154.47	-36.67	-38.15	423.00	235.00
1122	R-115	No	C2CLF5	154.47	-36.67	-38.15	423.00	235.00
1123	STYRENE	No	C8H8	104.14	293.25	145.14	752.92	418.29
1124	ALLYL CHLORIDE	No	C3H5CL	76.53	113.27	45.15	572.94	318.30
1124	3-CHLORO-1-PROPENE	No	C3H5CL	76.53	113.27	45.15	572.94	318.30
1125	BROMOMETHANE	No	CH3BR	94.94	38.41	3.56	498.08	276.71
1125	METHYL BROMIDE	No	CH3BR	94.94	38.41	3.56	498.08	276.71
1126	IODOMETHANE	No	CH3I	141.94	108.37	42.43	568.04	315.58
1126	METHYL IODODE	No	CH3I	141.94	108.37	42.43	568.04	315.58
1127	1,2-DICHLOROENZENE	No	C6H4CL2	147.01	356.76	180.42	816.43	453.57
1127	O-DICHLOROENZENE	No	C6H4CL2	147.01	356.76	180.42	816.43	453.57
1128	3-METHYL PYRIDINE	No	C6H7N	93.13	291.45	144.14	751.12	417.29
1128	3-PICOLINE	No	C6H7N	93.13	291.45	144.14	751.12	417.29

## Chapter 2

1129	1-HEPTANOL	No	C7H16O	116.19	349.16	176.20	808.83	449.35
1129	HEPTYL ALCOHOL	No	C7H16O	116.19	349.16	176.20	808.83	449.35
1130	1-OCTANOL	No	C8H18O	130.22	383.36	195.20	843.03	468.35
1130	OCTYL ALCOHOL	No	C8H18O	130.22	383.36	195.20	843.03	468.35
1131	AMYL CHLORIDE	No	C5H11CL	106.59	225.92	107.73	685.59	380.88
1131	1-CHLOROPENTANE	No	C5H11CL	106.59	225.92	107.73	685.59	380.88
1132	ALLYL ALCOHOL	No	C3H6O	58.08	205.97	96.65	665.64	369.80
1133	ACETALDEHYDE	No	C2H4O	44.05	68.27	20.15	527.94	293.30
1134	METHYL PROPYL ETHER	No	C4H10O	74.12	102.29	39.05	561.96	312.20
1135	DIPROPYL ETHER	No	C6H14O	102.17	194.09	90.05	653.76	363.20
1135	PROPYL ETHER	No	C6H14O	102.17	194.09	90.05	653.76	363.20
1136	BUTYL CHLORIDE	No	C4H9CL	92.57	173.21	78.45	632.88	351.60
1136	1-CHLOROBUTANE	No	C4H9CL	92.57	173.21	78.45	632.88	351.60
1137	CHLOROETHENE	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1137	CHLOROETHYLENE	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1137	VINYL CHLORIDE	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1137	REFRIGERANT 1140	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1137	R1140	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1137	R-1140	No	C2H3CL	62.50	7.16	-13.80	466.83	259.35
1138	CIS-1,2-DICHLOROETHENE	No	C2H2CL2	96.95	139.73	59.85	599.40	333.00
1138	1,2-DICHLOROETHYLENE,CIS	No	C2H2CL2	96.95	139.73	59.85	599.40	333.00
1139	TRANS-1,2-DICHLOROETHENE	No	C2H2CL2	96.95	117.77	47.65	577.44	320.80
1139	1,2-DICHLOROETHYLENE,TRANS	No	C2H2CL2	96.95	117.77	47.65	577.44	320.80
1139	REFRIGERANT 1130	No	C2H2CL2	96.95	117.77	47.65	577.44	320.80
1139	R1130	No	C2H2CL2	96.95	117.77	47.65	577.44	320.80
1139	R-1130	No	C2H2CL2	96.95	117.77	47.65	577.44	320.80
1140	TRICHLOROETHENE	No	C2HCL3	131.39	188.51	86.95	648.18	360.10
1140	TRICHLOROETHYLENE	No	C2HCL3	131.39	188.51	86.95	648.18	360.10
1140	REFRIGERANT 1120	No	C2HCL3	131.39	188.51	86.95	648.18	360.10
1140	R1120	No	C2HCL3	131.39	188.51	86.95	648.18	360.10
1140	R-1120	No	C2HCL3	131.39	188.51	86.95	648.18	360.10
1141	1-BROMOPROPANE	No	C3H7BR	123.00	159.80	71.00	619.47	344.15
1142	1-BROMOBUTANE	No	C4H9BR	137.02	214.88	101.60	674.55	374.75
1143	AMYL BROMIDE	No	C5H11BR	151.05	265.23	129.57	724.90	402.72
1143	1-BROMOPENTANE	No	C5H11BR	151.05	265.23	129.57	724.90	402.72
1144	ETHYL IODIDE	No	C2H5I	155.97	162.23	72.35	621.90	345.50
1144	IODOETHANE	No	C2H5I	155.97	162.23	72.35	621.90	345.50
1145	1-IODOPROPANE	No	C3H7I	169.99	216.41	102.45	676.08	375.60
1146	ETHYL METHYL SULFIDE	No	C3H8S	76.16	151.97	66.65	611.64	339.80
1147	BUTYL SULFIDE	No	C8H18S	146.29	372.03	188.91	831.70	462.06
1148	1-PROPANETHIOL	No	C3H8S	76.16	153.89	67.72	613.56	340.87
1148	PROPYL MERCAPTAN	No	C3H8S	76.16	153.89	67.72	613.56	340.87
1149	1-BUTANETHIOL	No	C4H10S	90.19	209.22	98.46	668.89	371.61
1149	BUTYL MERCAPTAN	No	C4H10S	90.19	209.22	98.46	668.89	371.61
1150	1-PENTANETHIOL	No	C5H12S	104.21	259.95	126.64	719.62	399.79
1150	PENTYL MERCAPTAN	No	C5H12S	104.21	259.95	126.64	719.62	399.79
1151	CYANOGEN	No	C2N2	52.04	-5.80	-21.00	453.87	252.15
1151	OXALIC ACID DINITRILE	No	C2N2	52.04	-5.80	-21.00	453.87	252.15
1152	CUMENE	No	C9H12	120.20	306.30	152.39	765.97	425.54
1152	ISOPROPYLBENZENE	No	C9H12	120.20	306.30	152.39	765.97	425.54
1153	FLUOROTRICHLOROMETHANE	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1153	REFRIGERANT 11	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1153	FREON 11	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1153	R11	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1153	TRICHLOROFLUOROMETHANE	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1153	R-11	No	CCL3F	137.37	74.48	23.60	534.15	296.75
1154	CHLORODIFLUOROMETHANE	No	CHCLF2	86.47	-41.44	-40.80	418.23	232.35
1154	REFRIGERANT 22	No	CHCLF2	86.47	-41.44	-40.80	418.23	232.35
1154	FREON 22	No	CHCLF2	86.47	-41.44	-40.80	418.23	232.35
1154	R22	No	CHCLF2	86.47	-41.44	-40.80	418.23	232.35
1154	R-22	No	CHCLF2	86.47	-41.44	-40.80	418.23	232.35
1155	CHLOROTRIFLUOROMETHANE	No	CCLF3	104.46	-113.98	-81.10	345.69	192.05
1155	REFRIGERANT 13	No	CCLF3	104.46	-113.98	-81.10	345.69	192.05
1155	FREON 13	No	CCLF3	104.46	-113.98	-81.10	345.69	192.05
1155	R13	No	CCLF3	104.46	-113.98	-81.10	345.69	192.05
1155	R-13	No	CCLF3	104.46	-113.98	-81.10	345.69	192.05
1156	CYCLOPROPANE	Yes	C3H6	42.08	-27.04	-32.80	432.63	240.35
1156	RC270	Yes	C3H6	42.08	-27.04	-32.80	432.63	240.35
1156	TRIMETHYLENE	Yes	C3H6	42.08	-27.04	-32.80	432.63	240.35
1157	N-BUTYLBENZENE	No	C10H14	134.22	361.95	183.31	821.62	456.46
1157	1-PHENYLBUTANE	No	C10H14	134.22	361.95	183.31	821.62	456.46



# Database Components

1158	BIPHENYL	No	C12H10	154.21	490.91	254.95	950.58	528.10
1158	PHENYL BENZENE	No	C12H10	154.21	490.91	254.95	950.58	528.10
1159	ISOHEXANE	Yes	C6H14	86.17	140.49	60.27	600.16	333.42
1159	2-METHYLPENTANE	Yes	C6H14	86.17	140.49	60.27	600.16	333.42
1160	2,3-DIMETHYLPENTANE	No	C7H16	100.20	193.61	89.78	653.28	362.93
1161	2,2,3-TRIMETHYLBUTANE	No	C7H16	100.20	177.59	80.88	637.26	354.03
1161	TRIPTANE	No	C7H16	100.20	177.59	80.88	637.26	354.03
1162	2,3-DIMETHYLHEXANE	No	C8H18	114.22	240.09	115.61	699.76	388.76
1163	2,4-DIMETHYLHEXANE	No	C8H18	114.22	228.97	109.43	688.64	382.58
1164	2,5-DIMETHYLHEXANE	No	C8H18	114.22	228.38	109.10	688.05	382.25
1165	3,4-DIMETHYLHEXANE	No	C8H18	114.22	243.91	117.73	703.58	390.88
1166	3-METHYLHEPTANE	No	C8H18	114.22	246.06	118.92	705.73	392.07
1167	4-METHYLHEPTANE	No	C8H18	114.22	243.88	117.71	703.55	390.86
1168	2,2,3-TRIMETHYLPENTANE	No	C8H18	114.22	229.71	109.84	689.38	382.99
1169	2,3,3-TRIMETHYLPENTANE	No	C8H18	114.22	238.57	114.76	698.24	387.91
1170	2,3,4-TRIMETHYLPENTANE	No	C8H18	114.22	236.24	113.47	695.91	386.62
1171	ARGON	Yes	AR	39.95	-302.54	-185.86	157.13	87.29
1172	HELIUM	Yes	HE	4.00	-452.10	-268.94	7.57	4.21
1173	NEON	No	NE	20.18	-410.95	-246.08	48.72	27.07
1174	KRYPTON	No	KR	83.80	-244.01	-153.34	215.66	119.81
1175	XENON	No	XE	131.30	-162.65	-108.14	297.02	165.01
1176	DICHLORODIFLUOROMETHANE	No	CCL2F2	120.91	-21.62	-29.79	438.05	243.36
1176	FREON 12	No	CCL2F2	120.91	-21.62	-29.79	438.05	243.36
1176	REFRIGERANT 12	No	CCL2F2	120.91	-21.62	-29.79	438.05	243.36
1176	R12	No	CCL2F2	120.91	-21.62	-29.79	438.05	243.36
1176	R-12	No	CCL2F2	120.91	-21.62	-29.79	438.05	243.36
1177	1,2-DIETHYLBENZENE	No	C10H14	134.22	362.22	183.46	821.89	456.61
1177	O-DIETHYLBENZENE	No	C10H14	134.22	362.22	183.46	821.89	456.61
1178	BROMINE	No	BR2	159.83	137.77	58.76	597.44	331.91
1179	3,3-DIMETHYL-1-BUTENE	No	C6H12	84.16	106.23	41.24	565.90	314.39
1180	2,3-DIMETHYL-1-BUTENE	No	C6H12	84.16	132.13	55.63	591.80	328.78
1181	2,3-DIMETHYL-2-BUTENE	No	C6H12	84.16	163.77	73.21	623.44	346.36
1181	TETRAMETHYLETHYLENE	No	C6H12	84.16	163.77	73.21	623.44	346.36
1182	ISOPROPYLACETYLENE	No	C5H8	68.11	79.43	26.35	539.10	299.50
1182	3-METHYL-1-BUTYNE	No	C5H8	68.11	79.43	26.35	539.10	299.50
1183	2,2-DIMETHYLPENTANE	No	C7H16	100.21	174.55	79.19	634.22	352.34
1184	3,3-DIMETHYLPENTANE	No	C7H16	100.21	186.92	86.07	646.59	359.22
1185	TRIETHYLMETHANE	No	C7H16	100.21	200.26	93.48	659.93	366.63
1185	3-ETHYLPENTANE	No	C7H16	100.21	200.26	93.48	659.93	366.63
1186	3-ETHYLHEXANE	No	C8H18	114.23	245.36	118.53	705.03	391.68
1187	2,2-DIMETHYLHEXANE	No	C8H18	114.23	224.39	106.88	684.06	380.03
1188	3,3-DIMETHYLHEXANE	No	C8H18	114.23	233.55	111.97	693.22	385.12
1189	2-METHYL-3-ETHYLPENTANE	No	C8H18	114.23	240.19	115.66	699.86	388.81
1190	3-METHYL-3-ETHYLPENTANE	No	C8H18	114.23	244.87	118.26	704.54	391.41
1191	HEXAMETHYLETHANE	No	C8H18	114.23	223.65	106.47	683.32	379.62
1191	2,2,3,3-TETRAMETHYLBUTANE	No	C8H18	114.23	223.65	106.47	683.32	379.62
1192	CYCLOHEPTANE	No	C7H14	98.18	245.26	118.48	704.93	391.63
1192	HEPTAMETHYLENE	No	C7H14	98.18	245.26	118.48	704.93	391.63
1192	SUBERANE	No	C7H14	98.18	245.26	118.48	704.93	391.63
1193	TRANS-1,2-DIMETHYLCYCLOHEXANE	No	C8H16	112.22	254.16	123.42	713.83	396.57
1194	2,2,3-TRIMETHYLHEXANE	No	C9H20	128.26	272.48	133.60	732.15	406.75
1195	3,3-DIETHYLPENTANE	No	C9H20	128.26	295.10	146.17	754.77	419.32
1195	TETRAETHYLMETHANE	No	C9H20	128.26	295.10	146.17	754.77	419.32
1196	2,2,3,3-TETRAMETHYLPENTANE	No	C9H20	128.26	284.49	140.27	744.16	413.42
1197	2,2,3,4-TETRAMETHYLPENTANE	No	C9H20	128.26	271.43	133.02	731.10	406.17
1198	2,2,4,4-TETRAMETHYLPENTANE	No	C9H20	128.26	252.11	122.28	711.78	395.43
1199	2,3,3,4-TETRAMETHYLPENTANE	No	C9H20	128.26	286.79	141.55	746.46	414.70
1200	1,4-DIETHYLBENZENE	No	C10H14	134.22	362.75	183.75	822.42	456.90
1200	P-DIETHYLBENZENE	No	C10H14	134.22	362.75	183.75	822.42	456.90
1201	DURENE	No	C10H14	134.21	386.23	196.79	845.90	469.94
1201	1,2,4,5-TETRAMETHYLBENZENE	No	C10H14	134.21	386.23	196.79	845.90	469.94
1202	3,3,5-TRIMETHYLHEPTANE	No	C10H22	142.27	312.22	155.68	771.89	428.83
1203	2,2,5,5-TETRAMETHYLHEXANE	No	C10H22	142.27	279.43	137.46	739.10	410.61
1204	1,1,1,2F4-ETHANE	No	C2F4H2	102.03	-14.90	-26.06	444.77	247.09
1204	FREON 134A	No	C2F4H2	102.03	-14.90	-26.06	444.77	247.09
1204	REFRIGERANT 134A	No	C2F4H2	102.03	-14.90	-26.06	444.77	247.09
1204	R134A	No	C2F4H2	102.03	-14.90	-26.06	444.77	247.09
1204	R-134A	No	C2F4H2	102.03	-14.90	-26.06	444.77	247.09
1205	22DICI-111F3-C2	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03
1205	FREON 123	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03
1205	REFRIGERANT 123	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03

## Chapter 2

1205	R123	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03
1205	R-123	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03
1205	2,2-DICHLORO-1,1,1-TRIFLUOROETHANE	No	C2CL2F3H	152.93	82.00	27.78	541.67	300.03
1206	DISILANE	No	H6Si2	62.22	5.90	-14.15	465.57	259.00
1206	SILICOETHANE	No	H6Si2	62.22	5.90	-14.15	465.57	259.00
1206	DISILICANE	No	H6Si2	62.22	5.90	-14.15	465.57	259.00
1207	TETRAFLUORSILANE	No	F4Si	104.08	-139.27	-95.15	320.40	178.00
1207	SILICON TETRAFLUORIDE	No	F4Si	104.08	-139.27	-95.15	320.40	178.00
1207	SILICON FLUORIDE	No	F4Si	104.08	-139.27	-95.15	320.40	178.00
1208	DICHLORSILANE	No	Cl2H2Si	101.01	46.94	8.30	506.61	281.45
1208	DICHLOROSILANE	No	Cl2H2Si	101.01	46.94	8.30	506.61	281.45
1209	TRICHLORSILANE	No	Cl3HSi	135.45	89.33	31.85	549.00	305.00
1209	TRICHLOROSILANE	No	Cl3HSi	135.45	89.33	31.85	549.00	305.00
1209	SILICOCHLOROFORM	No	Cl3HSi	135.45	89.33	31.85	549.00	305.00
1209	TRICHLOROMONOSILANE	No	Cl3HSi	135.45	89.33	31.85	549.00	305.00
1210	TETRACHLORSILANE	No	Cl4Si	169.90	134.33	56.85	594.00	330.00
1210	SILICON TETRACHLORIDE	No	Cl4Si	169.90	134.33	56.85	594.00	330.00
1210	TETRACHLOROSILANE	No	Cl4Si	169.90	134.33	56.85	594.00	330.00
1210	TETRACHLORO SILICON	No	Cl4Si	169.90	134.33	56.85	594.00	330.00
1210	SILICON CHLORIDE	No	Cl4Si	169.90	134.33	56.85	594.00	330.00
1215	NITROGEN DIOXIDE	No	NO2	46.01	69.80	38.78	529.47	294.15
1216	NITROGEN TETROXIDE	No	N2O4	92.01	70.09	38.94	529.76	294.31
1216	DINITROGEN TETRAOXIDE	No	N2O4	92.01	70.09	38.94	529.76	294.31
1216	DINITROGEN TETROXIDE	No	N2O4	92.01	70.09	38.94	529.76	294.31
1216	NITROGEN PEROXIDE	No	N2O4	92.01	70.09	38.94	529.76	294.31
1217	NITROGEN TRIOXIDE	No	N2O3	76.01	35.60	19.78	495.27	275.15
1217	DINITROGEN TRIOXIDE	No	N2O3	76.01	35.60	19.78	495.27	275.15
1218	DMPEG	No	C12H26O6	280.00	416.00	213.33	875.67	486.48
1218	DEPG	No	C12H26O6	280.00	416.00	213.33	875.67	486.48
1218	DMEPEG	No	C12H26O6	280.00	416.00	213.33	875.67	486.48
1218	COASTAL AGR SOLVENT	No	C12H26O6	280.00	416.00	213.33	875.67	486.48
1218	GENOSORB 1753	No	C12H26O6	280.00	416.00	213.33	875.67	486.48
1219	PIPERAZINE	Yes	C4H10N2	86.14	294.80	146.00	754.47	419.15
1219	PZ	Yes	C4H10N2	86.14	294.80	146.00	754.47	419.15
1220	PENTADECANOIC ACID	No	C15H30O2	242.40	642.02	338.90	1101.69	612.05
1220	PENTADECYLIC ACID	No	C15H30O2	242.40	642.02	338.90	1101.69	612.05
1221	LINOLEIC ACID	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	GRAPE SEED OIL	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	cis,cis-LINOLEIC ACID	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	EMERSOL 310-315	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	9,12-OCTADECADIENOIC ACID	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	LEINOLEIC ACID	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	9,12-LINOLEIC ACID	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	POLYLIN NO.515	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1221	PAMOLYN 200,240,380	No	C18H32O2	280.45	670.73	354.85	1130.40	628.00
1222	LINOLENIC ACID	No	C18H30O2	278.435	677.93	358.85	1137.60	632.00
1222	alpha-LINOLENIC ACID	No	C18H30O2	278.435	677.93	358.85	1137.60	632.00
1222	INDUSTRENE 120	No	C18H30O2	278.435	677.93	358.85	1137.60	632.00
1223	HEXADECANOIC ACID	No	C16H32O2	256.429	663.80	351.00	1123.47	624.15
1223	n-HEXADECANOIC ACID	No	C16H32O2	256.429	663.80	351.00	1123.47	624.15
1223	n-HEXADECANOIC ACID	No	C16H32O2	256.429	663.80	351.00	1123.47	624.15
1223	1-PENTADECANECARBOXYLIC ACID	No	C16H32O2	256.429	663.80	351.00	1123.47	624.15
1223	PALMITIC ACID	No	C16H32O2	256.429	663.80	351.00	1123.47	624.15
1224	PENTAFLUOROETHANE	No	C2HF5	120.022	-54.60	-48.11	405.07	225.04
1224	R-125	No	C2HF5	120.022	-54.60	-48.11	405.07	225.04
1224	R125	No	C2HF5	120.022	-54.60	-48.11	405.07	225.04
1224	REFRIGERANT 125	No	C2HF5	120.022	-54.60	-48.11	405.07	225.04
1225	HEXANOIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	BUTYLACETIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	HEXOIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	n-HEXOIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	PENTYLFORMIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	CAPROIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	n-CAPROIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1225	PENTANE-1-CARBOXYLIC ACID	No	C6H12O2	116.16	402.26	205.70	861.93	478.85
1226	HEPTANOIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	1-HEXANECARBOXYLIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	ENANTHYLIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	n-HEPTOIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	OENANTHIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	ENANTHIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15

## Database Components

1226	n-HEPTYLIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	OENANTHYLIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1226	HEPTHLIC ACID	No	C7H14O2	130.187	433.40	223.00	893.07	496.15
1227	OCTANOIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1227	n-CAPRYLIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1227	n-OCTOIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1227	1-HEPTANECARBOXYLIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1227	OCTIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1227	n-OCTYLIC ACID	No	C8H16O2	144.214	463.46	239.70	923.13	512.85
1228	NONANOIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	n-NONOIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	n-NONYLIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	PELARGIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	PELARGONIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	NONOIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	n-NONYLIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	PELARGIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	PELARGONIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	NONOIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	NONYLIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1228	1-OCTANECARBOXYLIC ACID	No	C9H18O2	158.241	492.08	255.60	951.75	528.75
1229	n-CAPRIC ACID	No	C10H20O2	172.268	518.00	270.00	977.67	543.15
1229	n-DECYLIC ACID	No	C10H20O2	172.268	518.00	270.00	977.67	543.15
1229	CAPRIC ACID	No	C10H20O2	172.268	518.00	270.00	977.67	543.15
1229	NONYLIC ACID	No	C10H20O2	172.268	518.00	270.00	977.67	543.15
1229	1-NONANECARBOXYLIC ACID	No	C10H20O2	172.268	518.00	270.00	977.67	543.15
1230	N-UNDECANOIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	CARBOXYLIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	UNDECYLIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	N-UNDECOIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	HENDECANOIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	1-DECANECARBOXYLIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1230	N-UNDECANOIC ACID	No	C11H22O2	186.294	543.56	284.20	1003.23	557.35
1231	N-DODECANOIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	DODECANOIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	DUODECYLIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	LAURIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	NEO-FAT 12	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	1-UNDECANECARBOXYLIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1231	LAUROSTEARIC ACID	No	C12H24O2	200.321	569.66	298.70	1029.33	571.85
1232	N-TRIDECANOIC ACID	No	C13H26O2	214.348	593.78	312.10	1053.45	585.25
1232	TRIDECANOIC ACID	No	C13H26O2	214.348	593.78	312.10	1053.45	585.25
1232	TRIDECYLIC ACID	No	C13H26O2	214.348	593.78	312.10	1053.45	585.25
1232	N-TRIDECOIC ACID	No	C13H26O2	214.348	593.78	312.10	1053.45	585.25
1233	N-TETRADECANOIC ACID	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	MYRISTIC ACID	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	CRODACID	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	HYDROFOL ACID 1495	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	1-TRIDECANECARBOXYLIC ACID	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	HYSTRENE 9014	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	N-TETRADECOIC ACID	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	EMERY 655	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1233	UNIVOL U 316S	No	C14H28O2	228.375	619.16	326.20	1078.83	599.35
1234	PENTADECANOIC ACID	No	C15H30O2	242.402	642.02	338.90	1101.69	612.05
1234	PENTADECYLIC ACID	No	C15H30O2	242.402	642.02	338.90	1101.69	612.05
1235	N-HEPTADECANOIC ACID	No	C17H34O2	270.456	684.68	362.60	1144.35	635.75
1235	HEPTADECANOIC ACID	No	C17H34O2	270.456	684.68	362.60	1144.35	635.75
1235	MARGARIC ACID	No	C17H34O2	270.456	684.68	362.60	1144.35	635.75
1235	N-HEPTADECYLIC ACID	No	C17H34O2	270.456	684.68	362.60	1144.35	635.75
1236	N-OCTADECANOIC ACID	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	OCTADECANOIC ACID	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	STEARIC ACID	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	1-HEPTADECANECARBOXYLIC ACID	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	NEO-FAT 18-61	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	STEAROPHANIC ACID	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1236	STEARIX BEADS	No	C18H36O2	284.483	707.36	375.20	1167.03	648.35
1237	NONADECANOIC ACID	No	C19H38O2	298.51	726.80	386.00	1186.47	659.15
1237	NONADECYLIC ACID	No	C19H38O2	298.51	726.80	386.00	1186.47	659.15
1238	N-EICOSANIC ACID	No	C20H40O2	312.536	746.60	397.00	1206.27	670.15
1238	ARACHIC ACID	No	C20H40O2	312.536	746.60	397.00	1206.27	670.15
1238	ARACHIDIC ACID	No	C20H40O2	312.536	746.60	397.00	1206.27	670.15

## Chapter 2

1238	EICOSANIC ACID	No	C20H40O2	312.536	746.60	397.00	1206.27	670.15
1239	OLEIC ACID	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1239	CIS-OCTADEC-9-ENOIC ACID	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1239	9,10-OCTADECENOIC ACID	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1239	PAMOLYN 100	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1239	CIS-9-OCTADECENOIC ACID	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1239	RED OIL	No	C18H34O2	282.467	679.73	359.85	1139.40	633.00
1240	CHLORODIFLUOROMETHANE	No	CHCLF2	86.47	-41.494	-40.83	418.176	232.32
1240	DIFLUOROCHLOROMETHANE	No	CHCLF2	86.47	-41.494	-40.83	418.176	232.32
1240	R-22	No	CHCLF2	86.47	-41.494	-40.83	418.176	232.32
1240	FREON 22	No	CHCLF2	86.47	-41.494	-40.83	418.176	232.32
1240	R22	No	CHCLF2	86.47	-41.494	-40.83	418.176	232.32
1241	DIFLUOROMETHANE	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	R-32	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	METHYLENE DIFLUORIDE	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	GENETRON 32	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	METHYLENE FLUORIDE	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	FREON 32	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1241	R32	No	CH2F2	52.02	-60.97	-51.65	398.7	221.50
1242	2-CHLORO-1,1,1,2-TETRAFLUOROETHANE	No	C2HCLF4	136.48	10.22	-12.10	469.89	261.05
1242	R-124	No	C2HCLF4	136.48	10.22	-12.10	469.89	261.05
1242	FREON 124	No	C2HCLF4	136.48	10.22	-12.10	469.89	261.05
1242	R124	No	C2HCLF4	136.48	10.22	-12.10	469.89	261.05
1243	1-CHLORO-1,1-DIFLUOROETHANE	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	GENETRON 101	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	REFRIGERANT 142B	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	FREON 142	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	FLUOROCARBON-142B	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	R-142B	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1243	R142B	No	C2H3CLF2	100.50	15.44	-9.20	475.11	263.95
1244	R-404A	No	C2F5H/C2F3H3/C2F4H2	97.6	-51.61	-46.45	408.06	226.70
1244	DuPont Suva 404A	No	C2F5H/C2F3H3/C2F4H3	97.6	-51.61	-46.45	408.06	226.70
1244	HP62	No	C2F5H/C2F3H3/C2F4H4	97.6	-51.61	-46.45	408.06	226.70
1244	R404A	No	C2F5H/C2F3H3/C2F4H5	97.6	-51.61	-46.45	408.06	226.70
1245	SODIUM CHLORIDE	No	NaCl	58.4425	2669.09	1465.05	3128.76	1738.20
1245	COMMON SALT	No	NaCl	58.4425	2669.09	1465.05	3128.76	1738.20
1245	SALT	No	NaCl	58.4425	2669.09	1465.05	3128.76	1738.20
1245	TABLE SALT	No	NaCl	58.4425	2669.09	1465.05	3128.76	1738.20
1246	DICHLOROSILANE	No	Cl2H2Si	101.007	46.94	8.30	506.61	281.45
1247	NITROGEN TRICHLORIDE	No	Cl3N	120.365	159.80	71.00	619.47	344.15
1247	AGENE	No	Cl3N	120.365	159.80	71.00	619.47	344.15
1247	TRICHLORAMINE	No	Cl3N	120.365	159.80	71.00	619.47	344.15
1247	TRICHLORIDE NITRIDE	No	Cl3N	120.365	159.80	71.00	619.47	344.15
1248	TETRACHLOROSILANE	No	Cl4Si	169.896	134.33	56.85	594.00	330.00
1248	SILICON TETRACHLORIDE	No	Cl4Si	169.896	134.33	56.85	594.00	330.00
1248	SILICON CHLORIDE	No	Cl4Si	169.896	134.33	56.85	594.00	330.00
1248	TETRACHLOROSILICON	No	Cl4Si	169.896	134.33	56.85	594.00	330.00
1249	HYDROXYLAMINE	No	H3NO	33.03	229.73	109.85	689.40	383.00
1249	OXAMMONIUM	No	H3NO	33.03	229.73	109.85	689.40	383.00
1250	SODIUM FLUORIDE	No	NaF	41.988	3109.23	1709.57	3568.90	1982.72
1250	FLORIDINE	No	NaF	41.988	3109.23	1709.57	3568.90	1982.72
1250	NAT. VILLIAUMITE	No	NaF	41.988	3109.23	1709.57	3568.90	1982.72
1251	NITROGEN TRIFLUORIDE	No	NF3	71.002	-200.31	-129.06	259.36	144.09
1251	NITROGEN FLUORIDE	No	NF4	71.002	-200.31	-129.06	259.36	144.09
1252	SULFURIC ACID	No	H2SO4	98.0795	638.33	336.85	1098.00	610.00
1252	HYDROGEN SULFATE	No	H2SO4	98.0795	638.33	336.85	1098.00	610.00
1252	SULPHURIC ACID	No	H2SO4	98.0795	638.33	336.85	1098.00	610.00
1252	DIPPING ACID	No	H2SO4	98.0795	638.33	336.85	1098.00	610.00
1252	VITRIOL OIL	No	H2SO4	98.0795	638.33	336.85	1098.00	610.00
1253	R-404A	No		97.6	-51.61	-46.45	408.06	226.70
1253	HP 62	No		97.6	-51.61	-46.45	408.06	226.70
1253	R404A	No		97.6	-51.61	-46.45	408.06	226.70
1253	DuPont Suva 404A	No		97.6	-51.61	-46.45	408.06	226.70
1254	R-409A	No		97.45	-29.56	-34.20	430.11	238.95
1254	DuPont Suva 409A	No		97.45	-29.56	-34.20	430.11	238.95
1254	R409A	No		97.45	-29.56	-34.20	430.11	238.95
1255	R-410A	No		72.58	-60.84	-51.58	398.83	221.57

# Database Components

1255	DuPont Suva 410A	No		72.58	-60.84	-51.58	398.83	221.57
1255	R410A	No		72.58	-60.84	-51.58	398.83	221.57
1256	R-507	No		98.9	-52.06	-46.70	407.61	226.45
1256	DuPont R-507	No		98.9	-52.06	-46.70	407.61	226.45
1256	R507	No		98.9	-52.06	-46.70	407.61	226.45
1257	NITROUS ACID	No	HNO2	47.014				
1257	NITROSYL HYDROXIDE	No	HNO2	47.014				
1258	PHOSPHORIC ACID	No	H3PO4	97.995	764.33	406.85	1224.00	680.00
1258	ORTHOPHOSPHORIC ACID	No	H4PO4	97.995	764.33	406.85	1224.00	680.00
1259	POTASSIUM IODIDE	No	KI	166.003	2452.73	1344.85	2912.40	1618.00
1260	SILICON DIOXIDE	No	SiO2	60.0843	4046.09	2230.05	4505.76	2503.20
1260	SILICA	No	SiO2	60.0843	4046.09	2230.05	4505.76	2503.20
1260	QUARTZ	No	SiO2	60.0843	4046.09	2230.05	4505.76	2503.20
1261	SULFUR DICHLORIDE	No	SCL2	102.971	139.28	59.60	598.95	332.75
1261	DICHLOROSULFANE	No	SCL2	102.971	139.28	59.60	598.95	332.75
1261	SULFUR CHLORIDE	No	SCL2	102.971	139.28	59.60	598.95	332.75
1261	CHLORINE SULFIDE	No	SCL2	102.971	139.28	59.60	598.95	332.75
1261	MONOSULFUR CHLORIDE	No	SCL2	102.971	139.28	59.60	598.95	332.75
1262	SILICON	No	SI	28.085	8826.53	4885.85	9286.20	5159.00
1263	TRIETHYL ALUMINUM	No	C6H15AL	114.167	761.00	405.00	1220.67	678.15
1263	TEA	No	C6H15AL	114.167	761.00	405.00	1220.67	678.15
1264	FORMAMIDE	No	CH3NO	45.041	427.73	219.85	887.40	493.00
1264	CARBAMALDEHYDE	No	CH3NO	45.041	427.73	219.85	887.40	493.00
1264	METHANAMIDE	No	CH3NO	45.041	427.73	219.85	887.40	493.00
1265	1,1-DICHLOROETHYLENE	No	C2H2CL2	96.943	88.81	31.56	548.48	304.71
1265	1,1-DICHLOROETHENE	No	C2H2CL2	96.943	88.81	31.56	548.48	304.71
1265	VINYLDENE DICHLORIDE	No	C2H2CL2	96.943	88.81	31.56	548.48	304.71
1266	METHYL ISOCYANATE	No	C2H3NO	57.052	101.93	38.85	561.60	312.00
1266	METHYL ESTER ISOCYANIC ACID	No	C2H3NO	57.052	101.93	38.85	561.60	312.00
1266	ISO-CYANOMETHANE	No	C2H3NO	57.052	101.93	38.85	561.60	312.00
1266	METHYL CARBONIMIDE	No	C2H3NO	57.052	101.93	38.85	561.60	312.00
1267	DICYANDIAMIDE	No	C2H4N4	84.081	586.13	307.85	1045.80	581.00
1267	CYANOQUANIDINE	No	C2H4N4	84.081	586.13	307.85	1045.80	581.00
1267	GUANIDINECARBONITRILE	No	C2H4N4	84.081	586.13	307.85	1045.80	581.00
1267	DICYANODIAMIDE	No	C2H4N4	84.081	586.13	307.85	1045.80	581.00
1267	1-CYANOQUANIDINE	No	C2H4N4	84.081	586.13	307.85	1045.80	581.00
1268	PERACETIC ACID	No	C2H4O3	76.052	229.73	109.85	689.40	383.00
1268	ACETIC PEROXIDE	No	C2H4O3	76.052	229.73	109.85	689.40	383.00
1268	PEROXACETIC ACID	No	C2H4O3	76.052	229.73	109.85	689.40	383.00
1268	ACETYL HYDROPEROXIDE	No	C2H4O3	76.052	229.73	109.85	689.40	383.00
1268	PEROXYACETIC ACID	No	C2H4O3	76.052	229.73	109.85	689.40	383.00
1269	GLYCINE	No	C2H5NO2	75.067	798.53	425.85	1258.20	699.00
1269	AMINOACETIC ACID	No	C2H5NO2	75.067	798.53	425.85	1258.20	699.00
1269	GLYCOLIXIR	No	C2H5NO2	75.067	798.53	425.85	1258.20	699.00
1269	2,3-DIHYDROXYPROPIONIC ACID	No	C2H5NO2	75.067	798.53	425.85	1258.20	699.00
1270	PROPARGYL ALCOHOL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	2-PROPYN-1-OL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	ETHYNYL CARBINOL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	2-PROPYNOL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	PROPYNOL ALCOHOL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	1-PROPYNE-3-OL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1270	3-PROPYNOL	No	C3H4O	56.064	236.48	113.60	696.15	386.75
1271	HEXAFLUOROPROPYLENE	No	C3F6	150.023	-21.28	-29.60	438.39	243.55
1271	PERFLUOROPROPYLENE	No	C3F6	150.023	-21.28	-29.60	438.39	243.55
1271	HEXAFLUOROPROPENE	No	C3F6	150.023	-21.28	-29.60	438.39	243.55
1271	PERFLUOROPROPENE	No	C3F6	150.023	-21.28	-29.60	438.39	243.55
1271	PERFLUORO-1-PROPENE	No	C3F6	150.023	-21.28	-29.60	438.39	243.55
1272	1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	No	C3HF7	170.03	2.55	-16.36	462.22	256.79
1272	2-H-HEPTAFLUOROPROPANE	No	C3HF7	170.03	2.55	-16.36	462.22	256.79
1272	REFRIGERANT 227	No	C3HF7	170.03	2.55	-16.36	462.22	256.79
1272	R227	No	C3HF7	170.03	2.55	-16.36	462.22	256.79
1272	R-227	No	C3HF7	170.03	2.55	-16.36	462.22	256.79
1273	1,1,1,2,3,3,3-HEXAFLUOROPROPANE	No	C3H2F6	152.039	43.25	6.25	502.92	279.40
1273	REFRIGERANT 236EA	No	C3H2F6	152.039	43.25	6.25	502.92	279.40
1273	R236EA	No	C3H2F6	152.039	43.25	6.25	502.92	279.40
1273	R-236EA	No	C3H2F6	152.039	43.25	6.25	502.92	279.40
1274	1,1,1,2,2-PENTAFLUOROPROPANE	No	C3H3F5	134.049	0.23	-17.65	459.90	255.50
1274	REFRIGERANT 245	No	C3H3F5	134.049	0.23	-17.65	459.90	255.50
1274	R245	No	C3H3F5	134.049	0.23	-17.65	459.90	255.50
1274	R-245	No	C3H3F5	134.049	0.23	-17.65	459.90	255.50
1275	2,2,2-TRIFLUOROETHYLDIFLUOROMETHYL	No	C3H3F5O	150.048	84.20	29.00	543.87	302.15

## Chapter 2

	ETHER							
1275	REFRIGERANT E245	No	C3H3F5O	150.048	84.20	29.00	543.87	302.15
1275	R-E245	No	C3H3F5O	150.048	84.20	29.00	543.87	302.15
1275	RE245	No	C3H3F5O	150.048	84.20	29.00	543.87	302.15
1275	2(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE	No	C3H3F5O	150.048	84.20	29.00	543.87	302.15
1276	PYRAZOLE	No	C3H4N2	68.078	368.60	187.00	828.27	460.15
1276	1,2-DIAZOLE	No	C3H4N2	68.078	368.60	187.00	828.27	460.15
1277	BETA-PROPIOLACTONE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1277	2-OXACYCLOBUTANONE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1277	3-HYDROXYPROPIONIC ACID LACTONE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1277	2-OXOXETANE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1277	PROPIOLACTONE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1277	2-OXETANONE	No	C3H4O2	72.064	323.60	162.00	783.27	435.15
1278	ETHYLENE CARBONATE	No	C3H4O3	88.063	478.76	248.20	938.43	521.35
1278	CARBONIC ACID	No	C3H4O3	88.063	478.76	248.20	938.43	521.35
1278	CYCLIC ETHYLENE ESTER	No	C3H4O3	88.063	478.76	248.20	938.43	521.35
1278	GLYCOL CARBONATE	No	C3H4O3	88.063	478.76	248.20	938.43	521.35
1278	1,2-DIOXOLAN-2-ONE	No	C3H4O3	88.063	478.76	248.20	938.43	521.35
1279	PYRUVIC ACID	No	C3H4O3	88.063	329.00	165.00	788.67	438.15
1279	2-OXY-PROPANOIC ACID	No	C3H4O3	88.063	329.00	165.00	788.67	438.15
1279	PYRORACEMIC ACID	No	C3H4O3	88.063	329.00	165.00	788.67	438.15
1279	2-OXOPROPIONIC ACID	No	C3H4O3	88.063	329.00	165.00	788.67	438.15
1280	ALPHA-EPICHLOROHYDRIN	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	CHLOROMETHYL OXIRANE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	1-CHLORO-2,3-EPOXYPROPANE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	1,2-EPOXY-3-CHLOROPROPANE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	2(CHLOROMETHYL)-OXIRANE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	ECH	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	2,3-EPOXYPROPYL CHLORIDE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1280	CHLORO-1,2-PROPYLENE OXIDE	No	C3H5CLO	92.525	245.30	118.50	704.97	391.65
1281	MELAMINE	No	C3H6N6	126.121	807.53	430.85	1267.20	704.00
1281	1,3,5-TRIAZIN-2,4,6-TRIAMINE	No	C3H6N6	126.121	807.53	430.85	1267.20	704.00
1281	CYANUROTRIAMIDE	No	C3H6N6	126.121	807.53	430.85	1267.20	704.00
1281	CYANURAMIDE	No	C3H6N6	126.121	807.53	430.85	1267.20	704.00
1281	CYANUROTRIAMINE	No	C3H6N6	126.121	807.53	430.85	1267.20	704.00
1282	2,3-EPOXY-1-PROPANOL	No	C3H6O2	74.079	320.90	160.50	780.57	433.65
1282	GLYCIDOL	No	C3H6O2	74.079	320.90	160.50	780.57	433.65
1282	OXIRANEMETHANOL	No	C3H6O2	74.079	320.90	160.50	780.57	433.65
1282	HYDROXYMETHYLOXIRANE	No	C3H6O2	74.079	320.90	160.50	780.57	433.65
1282	2,3-EPOXYPROPANOL	No	C3H6O2	74.079	320.90	160.50	780.57	433.65
1283	LACTIC ACID	No	C3H6O3	90.079	422.33	216.85	882.00	490.00
1283	2-HYDROXYPROPANOIC ACID	No	C3H6O3	90.079	422.33	216.85	882.00	490.00
1283	ACETONIC ACID	No	C3H6O3	90.079	422.33	216.85	882.00	490.00
1283	ALPHA-HYDROXYPROPIONIC ACID	No	C3H6O3	90.079	422.33	216.85	882.00	490.00
1283	ETHYLIDENELACTIC ACID	No	C3H6O3	90.079	422.33	216.85	882.00	490.00
1284	TRIMETHYLALUMINUM	No	C3H9AL	72.086	260.82	127.12	720.49	400.27
1284	TMA	No	C3H9AL	73.086	262.62	128.12	722.29	401.27
1285	3-AMINO-1-PROPANOL	No	C3H9NO	75.111	369.50	187.50	829.17	460.65
1285	3-PROPANOLAMINE	No	C3H9NO	75.111	369.50	187.50	829.17	460.65
1285	BETA-ALANINOL	No	C3H9NO	75.111	369.50	187.50	829.17	460.65
1285	3-AMINOPROPANOL	No	C3H9NO	75.111	369.50	187.50	829.17	460.65
1285	3-HYDROXYPROPYLAMINE	No	C3H9NO	75.111	369.50	187.50	829.17	460.65
1286	1,3-PROPANEDIAMINE	No	C3H10N2	74.1259	278.60	137.00	738.27	410.15
1286	PROPANE-1,3-DIAMINE	No	C3H10N2	74.1259	278.60	137.00	738.27	410.15
1286	1,3-PDA	No	C3H10N2	74.1259	278.60	137.00	738.27	410.15
1286	TRIMETHYLENEDIAMINE	No	C3H10N2	74.1259	278.60	137.00	738.27	410.15
1286	DIAMINOPROPANE	No	C3H10N2	74.1259	278.60	137.00	738.27	410.15
1287	TRIMETHOXSILANE	No	C3H10O3SI	122.196	183.83	84.35	643.50	357.50
1288	OCTAFLUORO-2-BUTENE	No	C4F8	200.031	26.98	-2.79	486.65	270.36
1288	PERFLUORO-2-BUTENE	No	C4F8	200.031	26.98	-2.79	486.65	270.36
1288	1,1,1,2,3,4,4,4-OCTAFLUORO-2-BUTENE	No	C4F8	200.031	26.98	-2.79	486.65	270.36
1288	PERFLUOROBUTENE	No	C4F8	200.031	26.98	-2.79	486.65	270.36
1289	DECAFLUOROBUTANE	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1289	PERFLUORO2BUTANE	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1289	REFRIGERANT 31-1B	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1289	PERFLUORO-N-BUTANE	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1289	R31-1B	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1289	R-31-1B	No	C4F10	238.028	28.40	-2.00	488.07	271.15
1290	FUMARONITRILE	No	C4H2N2	78.073	366.80	186.00	826.47	459.15
1290	(E)-2-BUTENEDINITRILE	No	C4H2N2	78.073	366.80	186.00	826.47	459.15

## Database Components

1290	TRANS-BUTENEDINITRILE	No	C4H2N2	78.073	366.80	186.00	826.47	459.15
1290	TRANS-DICYANOETHYLENE	No	C4H2N2	78.073	366.80	186.00	826.47	459.15
1291	MALEONITRILE	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1291	(Z)-2-BUTENEDINITRILE	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1291	CIS-2-BUTENEDINITRILE	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1291	MALEINSAEURE-DINITRIL	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1291	CIS-BUTENEDINITRILE	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1291	CIS-DICYANOETHYLENE	No	C4H2N2	78.073	425.93	218.85	885.60	492.00
1292	PYRAZINE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1292	1,4-DIAZINE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1292	PARADIAZINE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1292	1,4-DIAZABENZENE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1292	PIAZINE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1292	P-DIAZINE	No	C4H4N2	80.089	240.80	116.00	700.47	389.15
1293	PYRIDAZINE	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1293	1,2-DIAZINE	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1293	ORTHODIAZINE	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1293	1,2-DIAZABENZENE	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1293	PYRIDAZIN	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1293	O-DIAZINE	No	C4H4N2	80.089	406.40	208.00	866.07	481.15
1294	PYRIMIDINE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1294	1,3-DIAZINE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1294	METADIAZINE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1294	1,3-DIAZABENZENE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1294	MIAZINE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1294	M-DIAZINE	No	C4H4N2	80.089	254.75	123.75	714.42	396.90
1295	ACROLEIN CYANOHYDRIN	No	C4H5NO	83.09	370.13	187.85	829.80	461.00
1295	2-HYDROXY-3-BUTENENITRILE	No	C4H5NO	83.09	370.13	187.85	829.80	461.00
1295	2-HYDROXY-BUT-3-ENENITRILE	No	C4H5NO	83.09	370.13	187.85	829.80	461.00
1296	2,3-DIHYDROFURAN	No	C4H6O	70.091	130.10	54.50	589.77	327.65
1296	4,5-DIHYDROFURAN	No	C4H6O	70.091	130.10	54.50	589.77	327.65
1297	2,5-DIHYDROFURAN	No	C4H6O	70.091	150.53	65.85	610.20	339.00
1297	1-OXOLENE	No	C4H6O	70.091	150.53	65.85	610.20	339.00
1298	TRANS-CROTONALDEHYDE	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1298	TRANS-2-BUTENAL	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1298	CROTONIC ALDEHYDE	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1298	CROTONAL	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1298	CROTYLALDEHYDE	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1298	BETA-METHYLACROLEIN	No	C4H6O	70.091	216.00	102.22	675.67	375.37
1299	METHACROLEIN	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	ISOBUTENAL	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	2-METHYL-2-PROPENAL	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	2-METHYLENPROPANAL	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	METHACRYLALDEHYDE	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	ALPHA-METHYLACROLEIN	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1299	METHACRYLIC ALDEHYDE	No	C4H6O	70.091	154.40	68.00	614.07	341.15
1302	SULFUR 2	No	S2	64.13	832.41	444.67	1292.08	717.82
1303	SULFUR 3	No	S3	96.20	832.41	444.67	1292.08	717.82
1304	SULFUR 4	No	S4	128.26	832.41	444.67	1292.08	717.82
1305	SULFUR 5	No	S5	160.33	832.41	444.67	1292.08	717.82
1306	SULFUR 6	No	S6	192.40	832.41	444.67	1292.08	717.82
1307	SULFUR 7	No	S7	224.46	832.41	444.67	1292.08	717.82
1308	SULFUR 8	No	S8	256.53	832.41	444.67	1292.08	717.82
1400	2-BUTYNE-1,4-DIOL	No	C4H6O2	86.09	460.40	238.00	920.07	511.15
1400	1,4-BUTYNE-DIOL	No	C4H6O2	86.09	460.40	238.00	920.07	511.15
1400	1,4-DIHYDROXY-2-BUTYNE	No	C4H6O2	86.09	460.40	238.00	920.07	511.15
1400	BIS(HYDROXYMETHYL)ACETYLENE	No	C4H6O2	86.09	460.40	238.00	920.07	511.15
1401	METHACRYLIC ACID	No	C4H6O2	86.09	321.80	161.00	781.47	434.15
1401	2-METHYL-2PROPENOIC ACID	No	C4H6O2	86.09	321.80	161.00	781.47	434.15
1401	ALPHA-METHYLACRYLIC ACID	No	C4H6O2	86.09	321.80	161.00	781.47	434.15
1401	2-METHYLPROPENOIC ACID	No	C4H6O2	86.09	321.80	161.00	781.47	434.15
1402	ACETONE CYANOHYDRIN	No	C4H7NO	85.106	339.53	170.85	799.20	444.00
1402	2-HYDROXY-2-METHYL-PROPANENITRILE	No	C4H7NO	85.106	339.53	170.85	799.20	444.00
1402	2-METHYLLACTONITRILE	No	C4H7NO	85.106	339.53	170.85	799.20	444.00
1402	2-HYDROXY-2-METHYLPROPIONITRILE	No	C4H7NO	85.106	339.53	170.85	799.20	444.00
1402	ALPHA-HYDROXYISOBUTYRONITRILE	No	C4H7NO	85.106	339.53	170.85	799.20	444.00
1403	2-PYRROLIDONE	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1403	2-PYRROLIDINONE	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1403	GAMMA-AMINO BUTYRIC ACID LACTAM	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1403	GAMMA-AMINO BUTYROLACTAM	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1403	BUTYROLACTAM	No	C4H7NO	85.106	484.11	251.17	943.78	524.32

## Chapter 2

1403	4-AMINOBUTANOIC ACID	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1403	2-OXYPYRROLIDINE	No	C4H7NO	85.106	484.11	251.17	943.78	524.32
1404	1,2-EPOXYBUTANE	No	C4H8O	72.107	146.16	63.42	605.83	336.57
1404	ETHYLOXIRANE	No	C4H8O	72.107	146.16	63.42	605.83	336.57
1404	1-BUTENE OXIDE	No	C4H8O	72.107	146.16	63.42	605.83	336.57
1404	1,2-BUTYLENE OXIDE	No	C4H8O	72.107	146.16	63.42	605.83	336.57
1404	1,2-BUTENE OXIDE	No	C4H8O	72.107	146.16	63.42	605.83	336.57
1405	TERT-BUTYLAMINE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	2-METHYL-2-PROPANAMINE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	2-AMINOISOBUTANE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	1,1-DIMETHYLETHYLAMINE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	2-METHYL-2-PROPANAMINE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	2-AMINO-2-METHYLPROPANE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	2-METHYL-2-AMINOPROPANE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1405	TRIMETHYLAMINOMETHANE	No	C4H11N	73.138	111.92	44.40	571.59	317.55
1406	ETHYL CYANOACETATE	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	CYANOACETIC ACID ETHYL ESTER	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	ETHYL CYANOETHANOATE	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	ETHYL CYANACETATE	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	CYANOACETIC ACID ETHYL ESTER	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	MALONIC ACID ETHYL ESTER NITRILE	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1406	USAF KF-25	No	C5H7NO2	113.116	402.80	206.00	862.47	479.15
1407	ALLYL ACETATE	No	C5H8O2	100.117	219.20	104.00	678.87	377.15
1407	2-PROPENYL ESTER ACETIC ACID	No	C5H8O2	100.117	219.20	104.00	678.87	377.15
1407	ACETIC ACID ALLYL ESTER	No	C5H8O2	100.117	219.20	104.00	678.87	377.15
1407	PROPENYL ETHANOATE	No	C5H8O2	100.117	219.20	104.00	678.87	377.15
1407	3-ACETOXYPROPENE	No	C5H8O2	100.117	219.20	104.00	678.87	377.15
1408	GLUTARALDEHYDE	No	C5H8O2	100.117	370.40	188.00	830.07	461.15
1408	PENTANEDIAL	No	C5H8O2	100.117	370.40	188.00	830.07	461.15
1409	METHYL DIETHANOLAMINE	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	2,2'-(METHYLIMINO)BIS-ETHANOL	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	N-METHYLDIETHANOLAMINE	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	N-METHYL-2,2-IMINODIETHANOL	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	BIS(2-HYDROXYETHYL) METHYL AMINE	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	USAF DO-52	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	N-METHYLIMINODIETHANOL	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	2,2-METHYLIMINO)DIETHANOL	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1409	N-METHYLAMINODIGLYCOL	No	C5H13NO2	119.164	472.73	244.85	932.40	518.00
1411	TRIETHANOLAMINE	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	2,2',2"-NITRILOTRISETHANOL	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	2,2',2"-NITRILOTRIETHANOL	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	TRIETHANOLAMIN	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	2,2,2-NITRILOTRIETHANOL	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	TRI(HYDROXYETHYL)AMINE	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1411	TRIS(2-HYDROXYETHYL)AMINE	No	C6H15NO3	149.19	635.70	335.39	1095.37	608.54
1412	2-NORBORNENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	BICYCLO(2.2.1)HEPT-2-ENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	NORBORNYLENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	NORBORNENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	NORFENCHENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	NORCAMPHENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1412	3,6-ENDOMETHYLENE-CYCLOHEXENE	No	C7H10	94.156	203.90	95.50	663.57	368.65
1413	PHTHALIC ANHYDRIDE	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1413	1,3-ISOBENZOFURANDIONE	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1413	1,2-BENZENEDICARBOXYLIC ACID ANHYDRIDE	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1413	1,3-DIOXOPHTHALAN	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1413	1,3-PHTHALANDIONE	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1413	PHTHALIC ACID ANHYDRIDE	No	C8H4O3	148.118	544.10	284.50	1003.77	557.65
1414	4-CARBOXYBENZALDEHYDE	No	C8H6O3	150.134	803.93	428.85	1263.60	702.00
1414	4-FORMYLBENZOIC ACID	No	C8H6O3	150.134	803.93	428.85	1263.60	702.00
1414	BENZALDEHYDE-4-CARBOXYLIX ACID	No	C8H6O3	150.134	803.93	428.85	1263.60	702.00
1414	TEREPHTHALALDEHYDIC ACID	No	C8H6O3	150.134	803.93	428.85	1263.60	702.00
1414	4-CBA	No	C8H6O3	150.134	803.93	428.85	1263.60	702.00
1415	PHTHALIC ACID	No	C8H6O4	166.133	616.73	324.85	1076.40	598.00
1415	1,2-BENZENEDICARBOXYLIC ACID	No	C8H6O4	166.133	616.73	324.85	1076.40	598.00
1415	BENZEN-1,2-DICARBOXYLIC ACID	No	C8H6O4	166.133	616.73	324.85	1076.40	598.00
1415	O-DICARBOXYBENZENE	No	C8H6O4	166.133	616.73	324.85	1076.40	598.00
1415	O-BENZENEDICARBOXYLIC ACID	No	C8H6O4	166.133	616.73	324.85	1076.40	598.00
1416	TEREPHTHALIC ACID	No	C8H6O4	166.13	1037.93	1224.45	1497.60	832.00
1416	1,4-BENZENEDICARBOXYLIC ACID	No	C8H6O4	166.13	1037.93	1224.45	1497.60	832.00
1416	BENZEN-1,2-DICARBOXYLIC ACID	No	C8H6O4	166.13	1037.93	1224.45	1497.60	832.00



# Database Components

1416	P-BENZENEDICARBOXYLIC ACID	No	C8H6O4	166.13	1037.93	1224.45	1497.60	832.00
1416	P-PHTHALIC ACID	No	C8H6O4	166.13	1037.93	1224.45	1497.60	832.00
1417	ETHYLBENZENE HYDROPEROXIDE	No	C8H10O2	138.17	505.13	691.65	964.80	536.00
1417	1-PHENYLETHYL HYDROPEROXIDE	No	C8H10O2	138.17	505.13	691.65	964.80	536.00
1418	METHYLNORBORNENE	No	C8H12	108.18	242.60	429.12	702.27	390.15
1418	2-METHYL-BICYCLO(2.2.1)HEPT-2-ENE	No	C8H12	108.18	242.60	429.12	702.27	390.15
1418	2-METHYL-2-NORBORNENE	No	C8H12	108.18	242.60	429.12	702.27	390.15
1418	2-METHYLNORBORNENE	No	C8H12	108.18	242.60	429.12	702.27	390.15
1419	DI-N-BUTYL ETHER	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	1,1'-OXYBISBUTANE	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	BUTYL OXIDE	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	DIBUTYL OXIDE	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	1-BUTOXYBUTANE	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	DIBUTYL ETHER	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1419	N-BUTYL ETHER	No	C8H18O	130.23	285.80	472.32	745.47	414.15
1420	TETRAETHYLENE GLYCOL	No	C8H18O5	194.23	625.19	811.71	1084.86	602.70
1420	2,2'-(OXYBIS(2,1-ETHANEDILOYX))BIS-ETHANOL	No	C8H18O5	194.23	625.19	811.71	1084.86	602.70
1420	2,2'-(OXYBIS(ETHYLENEOXY))DIETHANOL TETRAGLYCOL	No	C8H18O5	194.23	625.19	811.71	1084.86	602.70
1421	N-OCTYLAMINE	No	C8H19N	129.25	355.28	541.80	814.95	452.75
1421	1-OCTANAMINE	No	C8H19N	129.25	355.28	541.80	814.95	452.75
1421	1-OCTYLAMINE	No	C8H19N	129.25	355.28	541.80	814.95	452.75
1421	1-AMINOCTANE	No	C8H19N	129.25	355.28	541.80	814.95	452.75
1422	DIISOBUTYLAMINE	No	C8H19N	129.25	282.20	468.72	741.87	412.15
1422	2-METHYL-N-(2-METHYLPROPYL)-1-PROPANAMINE	No	C8H19N	129.25	282.20	468.72	741.87	412.15
1423	TETRAETHYL LEAD	No	C8H20PB	323.45	392.00	578.52	851.67	473.15
1423	TETRAETHYL PLUMBANE	No	C8H20PB	323.45	392.00	578.52	851.67	473.15
1424	OCTAMETHYLTRISILOXANE	No	C8H24O2SI3	236.53	306.59	493.11	766.26	425.70
1424	MDM	No	C8H24O2SI3	236.53	306.59	493.11	766.26	425.70
1425	OCTAMETHYLCYCLOTETRASILOXANE	No	C8H24O4SI4	296.62	347.00	533.52	806.67	448.15
1425	D4	No	C8H24O4SI4	296.62	347.00	533.52	806.67	448.15
1426	2,4-TOLUENE DIISOCYANATE	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1426	2,4-DIISOCYANATOMETHYLBENZENE	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1426	2,4-DIISOCYANATO-1-METHYLBENZENE	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1426	2,4-DIISOCYANATOTOLUENE	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1426	METHYLPHENYLENE ISOCYANATE	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1426	METHYLPHENYLENE ESTER ISOCYANIC ACID	No	C9H6N2O2	174.16	483.75	670.27	943.42	524.12
1427	2-METHYL-1-OCTENE	No	C9H18	126.24	292.37	478.89	752.04	417.80
1428	7-METHYL-1-OCTENE	No	C9H18	126.24	275.00	461.52	734.67	408.15
1429	2-NONANONE	No	C9H18O	142.24	381.20	567.72	840.87	467.15
1429	METHYL HEPTYL KETONE	No	C9H18O	142.24	381.20	567.72	840.87	467.15
1429	HEPTYL METHYL KETONE	No	C9H18O	142.24	381.20	567.72	840.87	467.15
1429	NONAN-2-ONE	No	C9H18O	142.24	381.20	567.72	840.87	467.15
1430	5-NONANONE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1430	DIBUTYL KETONE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1430	BUTYL KETONE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1430	NONAN-2-ONE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1430	5-OXONONANE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1430	N-VALERONE	No	C9H18O	142.24	371.21	557.73	830.88	461.60
1431	2,2-DIMETHYLHEPTANE	No	C9H20	128.258	270.84	132.69	730.51	405.84
1432	2-METHYLOCTANE	No	C9H20	128.258	289.90	143.28	749.57	416.43
1433	4-METHYLOCTANE	No	C9H20	128.258	288.39	142.44	748.06	415.59
1434	2-NONANOL	No	C9H20O	144.257	389.30	198.50	848.97	471.65
1434	HEPTYL METHYL CARBINOL	No	C9H20O	144.257	389.30	198.50	848.97	471.65
1435	DIALLYL MALEATE	No	C10H12O4	196.203	476.33	246.85	936.00	520.00
1435	DI-2-PROPENYL ESTER-2-BUTENEDIOIC ACID (Z)	No	C10H12O4	196.203	476.33	246.85	936.00	520.00
1436	P-CYMENE	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	1-METHYL-4-(1-METHYLETHYL)-BENZENE	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	1-ISOPROPYL-4-METHYLBENZENE	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	P-ISOPROPYLTOLUENE	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	CAMPHOGEN	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	CYMOL	No	C10H14	134.221	350.83	177.13	810.50	450.28
1436	P-METHYLISOPROPYLBENZENE	No	C10H14	134.221	350.83	177.13	810.50	450.28
1437	ADAMANTANE	No	C10H16	136.237	370.13	187.85	829.80	461.00
1437	TRICYCLO(3.3.1.1(3,7))DECANE	No	C10H16	136.237	370.13	187.85	829.80	461.00
1438	ETHYLENEDIAMINETETRAACETIC ACID	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15
1438	N,N'-1,2-ETHANEDIYLBIS(N-(CARBOXYMETHYL)-	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15

## Chapter 2

	GLYCINE							
1438	EDEIC ACID	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15
1438	EDTA ACID	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15
1438	ETHYLENEDINITRILOTETRAACETIC ACID	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15
1438	N,N,N',N'-ETHYLENEDIAMINETETRAACETIC ACID	No	C10H16N2O8	292.246	730.40	388.00	1190.07	661.15
1439	1-DECYNE	No	C10H18	138.253	345.20	174.00	804.87	447.15
1439	DEC-1-YNE	No	C10H18	138.253	345.20	174.00	804.87	447.15
1439	OCTYLACETYLENE	No	C10H18	138.253	345.20	174.00	804.87	447.15
1440	CIS-2-DECENE	No	C10H20	140.269	344.93	173.85	804.60	447.00
1440	(Z)-2-DECENE	No	C10H20	140.269	344.93	173.85	804.60	447.00
1441	TRANS-2-DECENE	No	C10H20	140.269	343.13	172.85	802.80	446.00
1441	(E)-2-DECENE	No	C10H20	140.269	343.13	172.85	802.80	446.00
1442	8-METHYL-1-NONENE	No	C10H20	140.269	338.90	170.50	798.57	443.65
1443	2-METHYLNONANE	No	C10H22	142.285	332.60	167.00	792.27	440.15
1444	8-METHYL-1-NONANOL	No	C10H22O	158.284	427.73	219.85	887.40	493.00
1444	ISODECYL ALCOHOL	No	C10H22O	158.284	427.73	219.85	887.40	493.00
1444	ISODECANOL	No	C10H22O	158.284	427.73	219.85	887.40	493.00
1445	ETHYLENE GLYCOL 2-ETHYLHEXYL ETHER	No	C10H22O2	174.283	442.40	228.00	902.07	501.15
1445	EG 2-ETHYLHEXYL ETHER	No	C10H22O2	174.283	442.40	228.00	902.07	501.15
1445	2-(2-ETHYLHEXYLOXY)-ETHANOL	No	C10H22O2	174.283	442.40	228.00	902.07	501.15
1446	DIPROPYLENE GLYCOL T-BUTYL ETHER	No	C10H22O3	190.283	467.33	241.85	927.00	515.00
1446	DI-PG-T-BUTYL ETHER	No	C10H22O3	190.283	467.33	241.85	927.00	515.00
1447	DEG-N-HEXYL EHTER	No	C10H22O3	190.283	771.53	410.85	1231.20	684.00
1447	2-(2-HEXOXYETHOXY)ETHANOL	No	C10H22O3	190.283	771.53	410.85	1231.20	684.00
1447	DIETHYLENE GLYCOL-N-HEXYL EHTER	No	C10H22O3	190.283	771.53	410.85	1231.20	684.00
1447	N-HEXYL CARBITOL	No	C10H22O3	190.283	771.53	410.85	1231.20	684.00
1447	3,6-DIOXODODECANOL-1	No	C10H22O3	190.283	771.53	410.85	1231.20	684.00
1448	TEG-N-BUTYL ETHER	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	2-(2-(2-BUTOXYETHOXY)ETHOXY)ETHANOL	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	TRIETHYLENE GLYCOL-N-HEXYL EHTER	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	BUTOXYTRYGLYCOL	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	TRIGLYCOL MONOBUTYL ETHER	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	BUTOXYTRIETHYLENE GLYCEROL	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1448	TRIETHYLENE GLYCOL BUTYL ETHER	No	C10H22O4	206.282	532.40	278.00	992.07	551.15
1449	TRI-PG-MONOMETHYL ETHER	No	C10H22O4	206.282	468.32	242.40	927.99	515.55
1449	TRIPROPYLENE GLYCOL MONOMETHYL ETHER	No	C10H22O4	206.282	468.32	242.40	927.99	515.55
1449	(2-(2-METHOXY-METHYLETHOXY)METHYL ETHOXY)-PROPAN-2-OL	No	C10H22O4	206.282	468.32	242.40	927.99	515.55
1449	(2-(2-METHOXYMETHYLETHOXY)METHYLETHOXY)-PROPANOL	No	C10H22O4	206.282	468.32	242.40	927.99	515.55
1450	TETRA-EG-DIMETHYL ETHER	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1450	TETRAETHYLENE GLYCOL DIMETHYL ETHER	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1450	DIMETHOXYTETRAGLYCOL	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1450	2,5,8,11,14-PENTAOXAPENTADECANE	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1450	TETRAGLYME	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1450	DIMETHOXYTETRAETHYLENEGLYCOL	No	C10H22O5	222.282	528.44	275.80	988.11	548.95
1451	P-ISOPROPENYLSTYRENE	No	C11H12	144.216	467.33	241.85	927.00	515.00
1451	1-ETHENYL-4-(1-METHYLETHENYL)-BENZENE	No	C11H12	144.216	467.33	241.85	927.00	515.00
1451	1-ISOPROPENYL-4-VINYL BENZENE	No	C11H12	144.216	467.33	241.85	927.00	515.00
1452	N-BUTYL BENZOATE	No	C11H14O2	178.231	482.00	250.00	941.67	523.15
1452	BUTYL ESTER BENZOIC ACID	No	C11H14O2	178.231	482.00	250.00	941.67	523.15
1453	1-ETHYL-2-ISOPROPYL BENZENE	No	C11H16	148.248	379.40	193.00	839.07	466.15
1453	1-ETHYL-2-(1-METHYLETHYL)-BENZENE	No	C11H16	148.248	379.40	193.00	839.07	466.15
1453	O-ETHYLCUMENE	No	C11H16	148.248	379.40	193.00	839.07	466.15
1454	PENTAMETHYLBENZENE	No	C11H16	148.248	448.52	231.40	908.19	504.55
1454	1,2,3,4,5-PENTAMETHYL BENZENE	No	C11H16	148.248	448.52	231.40	908.19	504.55
1455	P-TERT-AMYLPHENOL	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	4-(1,1-DIMETHYL PROPYL)-PHENOL	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	4-TERT-AMYLPHENOL	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	P-(1,1-DIMETHYL PROPYL)-PHENOL	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	R-T-PENTYL PHENOL	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	PENTAPHEN	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1455	1-HYDROXY-4-(2-METHYL-2-BUTYL)-BENZENE	No	C11H16O	164.247	504.50	262.50	964.17	535.65
1456	2-ETHYLHEXYL ACRYLATE	No	C11H20O2	184.279	420.80	216.00	880.47	489.15
1456	1-ETHYL-2-(1-METHYLETHYL)-BENZENE	No	C11H20O2	184.279	420.80	216.00	880.47	489.15
1456	O-ETHYLCUMENE	No	C11H20O2	184.279	420.80	216.00	880.47	489.15
1457	DIBENZOFURAN	No	C12H8O	168.195	545.29	285.16	1004.96	558.31
1457	DIPHENYLENE OXIDE	No	C12H8O	168.195	545.29	285.16	1004.96	558.31
1457	DIBENZOFURANE	No	C12H8O	168.195	545.29	285.16	1004.96	558.31

## Database Components

1458	BENZIDINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	(1,1'-BIPHENYL)-4,4'-DIAMINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	4,4'-DIAMINOBIPHENYL	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	P,P'-BIANILINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	4,4'-BIPHENYLDIAMINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	P,P'-DIANILINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	C.I. 37225	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	P-DIAMINODIPHENYL	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	P,P'-DIAMINOBIPHENYL	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	4,4'-BIANILINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	4,4'-BIPHENYLDIAMINE	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	C.I. AZOIC DIAZO COMPONENT 112	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	C.I. 37225	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1458	4,4'-DIAMINODIPHENYL	No	C12H12N2	184.241	755.06	401.70	1214.73	674.85
1459	DIETHYL PHTHALATE	No	C12H14O4	222.241	561.20	294.00	1020.87	567.15
1459	DIETHYL ESTER 1,2-BENZENEDICARBOXYLIC ACID	No	C12H14O4	222.241	561.20	294.00	1020.87	567.15
1459	DIETHYL-O-PHTHALATE	No	C12H14O4	222.241	561.20	294.00	1020.87	567.15
1459	DIETHYL-1,2-BENZENEDICARBOXYLATE	No	C12H14O4	222.241	561.20	294.00	1020.87	567.15
1459	ETHYL PHTHALATE	No	C12H14O4	222.241	561.20	294.00	1020.87	567.15
1460	P-TERT-BUTYLSTYRENE	No	C12H16	160.259	440.33	226.85	900.00	500.00
1460	1-(1,1-DIMETHYLETHYL)-4-ETHENYL-BENZENE	No	C12H16	160.259	440.33	226.85	900.00	500.00
1460	4-TERT-BUTYLSTYRENE	No	C12H16	160.259	440.33	226.85	900.00	500.00
1460	4-TERT-BUTYL VINYL BENZENE	No	C12H16	160.259	440.33	226.85	900.00	500.00
1461	CYCLOHEXYLBENZENE	No	C12H16	160.259	464.22	240.12	923.89	513.27
1461	PHENYLCYCLOHEXANE	No	C12H16	160.259	464.22	240.12	923.89	513.27
1462	P-ISOBUTYLSTYRENE	No	C12H16	160.259	483.53	250.85	943.20	524.00
1462	4-ISOBUTYLSTYRENE	No	C12H16	160.259	483.53	250.85	943.20	524.00
1462	1-ETHENYL-4-(2-METHYLPROPYL)-BENZENE	No	C12H16	160.259	483.53	250.85	943.20	524.00
1462	1-ISOBUTYL-4-VINYL-BENZENE	No	C12H16	160.259	483.53	250.85	943.20	524.00
1463	HEXAMETHYLBENZENE	No	C12H18	162.275	506.21	263.45	965.88	536.60
1463	1,2,3,4,5,6-HEXAMETHYLBENZENE	No	C12H18	162.275	506.21	263.45	965.88	536.60
1463	MELLITENE	No	C12H18	162.275	506.21	263.45	965.88	536.60
1464	N-HEXYLBENZENE	No	C12H18	162.275	439.00	226.11	898.67	499.26
1464	HEXYLBENZENE	No	C12H18	162.275	439.00	226.11	898.67	499.26
1464	1-PHENYLHEXANE	No	C12H18	162.275	439.00	226.11	898.67	499.26
1465	1,2,3-TRIETHYLBENZENE	No	C12H18	162.275	423.59	217.55	883.26	490.70
1466	1,2,4-TRIETHYLBENZENE	No	C12H18	162.275	424.40	218.00	884.07	491.15
1467	DIBUTYL MALEATE	No	C12H20O4	228.288	536.00	280.00	995.67	553.15
1467	BUTYL MALEATE	No	C12H20O4	228.288	536.00	280.00	995.67	553.15
1467	DIBUTYL ESTER-2-BUTENEDIOIC ACID	No	C12H20O4	228.288	536.00	280.00	995.67	553.15
1468	CIS-2-DODECENE	No	C12H24	168.323	424.13	217.85	883.80	491.00
1468	(Z)-2-DODECENE	No	C12H24	168.323	424.13	217.85	883.80	491.00
1469	TRANS-2-DODECENE	No	C12H24	168.323	424.13	217.85	883.80	491.00
1469	(E)-2-DODECENE	No	C12H24	168.323	424.13	217.85	883.80	491.00
1470	1-DODECANAL	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	DODECANAL	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	LAURIC C-12 ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	DODECYL ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	DUODECYL ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	N-LAURALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	LAURYL ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	N-DODECANAL	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	1-DODECYL ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	LAURALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1470	N-DODECYL ALDEHYDE	No	C12H24O	184.322	482.00	250.00	941.67	523.15
1471	3-METHYLBUNDECANE	No	C12H26	170.338	411.44	210.80	871.11	483.95
1472	DI-N-HEXYL ETHER	No	C12H26O	186.338	438.26	225.70	897.93	498.85
1472	1,1'-OXYBIS-HEXANE	No	C12H26O	186.338	438.26	225.70	897.93	498.85
1472	BIS(1-HEXYL)ETHER	No	C12H26O	186.338	438.26	225.70	897.93	498.85
1472	HEXYL ETHER	No	C12H26O	186.338	438.26	225.70	897.93	498.85
1473	N-DODECYLAMINE	No	C12H27N	185.353	498.56	259.20	958.23	532.35
1473	1-DODECANAMINE	No	C12H27N	185.353	498.56	259.20	958.23	532.35
1473	DODECYLAMINE	No	C12H27N	185.353	498.56	259.20	958.23	532.35
1473	1-AMINODODECANE	No	C12H27N	185.353	498.56	259.20	958.23	532.35
1473	LAURYLAMINE	No	C12H27N	185.353	498.56	259.20	958.23	532.35
1474	BENZOPHENONE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1474	DIPHENYL KETONE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1474	DIPHENYL METHANONE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1474	Synonym3=BENZOYLBENZENE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1474	Synonym4=ALPHA-OXODIPHENYLMETHANE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24

## Chapter 2

1474	Synonym5=PHENYL KETONE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1474	ALPHA-OXODITANE	No	C13H10O	182.222	582.96	306.09	1042.63	579.24
1475	N-HEPTYLBENZENE	No	C13H20	176.302	474.98	246.10	934.65	519.25
1475	HEPTYLBENZENE	No	C13H20	176.302	474.98	246.10	934.65	519.25
1475	1-HEPTYLBENZENE	No	C13H20	176.302	474.98	246.10	934.65	519.25
1475	1-PHENYLHEPTANE	No	C13H20	176.302	474.98	246.10	934.65	519.25
1476	N-BUTYL NONANOATE	No	C13H26O2	214.348	476.33	246.85	936.00	520.00
1476	BUTYL ESTER NONANOIC ACID	No	C13H26O2	214.348	476.33	246.85	936.00	520.00
1476	BUTYL PELARGONATE	No	C13H26O2	214.348	476.33	246.85	936.00	520.00
1477	DIPHENYLACETYLENE	No	C14H10	178.233	571.73	299.85	1031.40	573.00
1477	TOLANE	No	C14H10	178.233	571.73	299.85	1031.40	573.00
1477	1,1'-(1,2-ETHYNYLDIYL)BIS-BENZENE	No	C14H10	178.233	571.73	299.85	1031.40	573.00
1478	CIS-STILBENE	No	C14H12	180.249	537.53	280.85	997.20	554.00
1478	(Z)-1,1'-(1,2-ETHENEDIYL)BIS-BENZENE	No	C14H12	180.249	537.53	280.85	997.20	554.00
1478	(Z)-1,2-DIPHENYLETHENE	No	C14H12	180.249	537.53	280.85	997.20	554.00
1478	CIS-DIBENZAL	No	C14H12	180.249	537.53	280.85	997.20	554.00
1478	CIS-TOLUYLENE	No	C14H12	180.249	537.53	280.85	997.20	554.00
1478	CIS-DIBENZILIDENE	No	C14H12	180.249	537.53	280.85	997.20	554.00
1479	TRANS-STILBENE	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1479	(E)-1,1'-(1,2-ETHENEDIYL)BIS-BENZENE	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1479	(E)-1,2-DIPHENYLETHENE	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1479	TRANS-DIBENZAL	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1479	TRANS-TOLUYLENE	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1479	TRANS-DIBENZILIDENE	No	C14H12	180.249	583.70	306.50	1043.37	579.65
1480	BENZYL BENZOATE	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1480	BENZYL ESTER	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1480	PHENYLMETHYL ESTER BENZOIC ACID	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1480	BENZYL ESTER BENZOIC ACID	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1480	BENZYL BENZENECARBOXYLATE	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1480	BENZYL PHENYLFORMATE	No	C14H12O2	212.248	613.83	323.24	1073.50	596.39
1481	1,1-DIPHENYLETHANE	No	C14H14	182.265	522.73	272.63	982.40	545.78
1481	1,1'-ETHYLDIBISBENZENE	No	C14H14	182.265	522.73	272.63	982.40	545.78
1481	ALPHA-METHYLDIPHENYLMETHANE	No	C14H14	182.265	522.73	272.63	982.40	545.78
1482	1,2-DIPHENYLETHANE	No	C14H14	182.265	536.90	280.50	996.57	553.65
1482	(PHENYLETHYL)BENZENE	No	C14H14	182.265	536.90	280.50	996.57	553.65
1482	BIBENZYL	No	C14H14	182.265	536.90	280.50	996.57	553.65
1482	DIBENZYL	No	C14H14	182.265	536.90	280.50	996.57	553.65
1483	DIBENZYL ETHER	No	C14H14O	198.265	550.94	288.30	1010.61	561.45
1483	1,1'-(OXYBIS(METHYLENE))BIS-BENZENE	No	C14H14O	198.265	550.94	288.30	1010.61	561.45
1483	BENZYL ETHER	No	C14H14O	198.265	550.94	288.30	1010.61	561.45
1483	DIBENZYL OXIDE	No	C14H14O	198.265	550.94	288.30	1010.61	561.45
1483	BENZYL OXIDE	No	C14H14O	198.265	550.94	288.30	1010.61	561.45
1484	1-BUTYLNAPHTHALENE	No	C14H16	184.281	552.90	289.39	1012.57	562.54
1484	1-N-BUTYLNAPHTHALENE	No	C14H16	184.281	552.90	289.39	1012.57	562.54
1484	ALPHA-BUTYLNAPHTHALENE	No	C14H16	184.281	552.90	289.39	1012.57	562.54
1484	1-NAPHTHYL-1-BUTANE	No	C14H16	184.281	552.90	289.39	1012.57	562.54
1485	2,6-DIETHYLNAPHTHALENE	No	C14H16	184.281	577.13	302.85	1036.80	576.00
1486	DIAMANTANE	No	C14H20	188.313	492.53	255.85	952.20	529.00
1486	DECAHYDRO-3,5,1,7-(1,2,3,4)BUTANETETRAYLNAPHTHALENE	No	C14H20	188.313	492.53	255.85	952.20	529.00
1486	CONGRESSANE	No	C14H20	188.313	492.53	255.85	952.20	529.00
1487	N-OCTYLBENZENE	No	C14H22	190.329	507.92	264.40	967.59	537.55
1488	1,2,3,5-TETRAETHYLBENZENE	No	C14H22	190.329	479.93	248.85	939.60	522.00
1489	PHENYLINDENE	No	C15H12	192.26	638.33	336.85	1098.00	610.00
1490	BISPHENOL A	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	4,4'-(1-METHYLETHYLIDENE)BIS-PHENOL	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	DIPHENYLOLPROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	2,2-BIS(4-HYDROXYPHENYL)PROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	2,2-BIS(P-HYDROXYPHENYL)PROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	4,4'-DIHYDROXYDIPHENYLPROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	4,4'-DIHYDROXY-2,2-DIPHENYLPROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1490	P,P'-DIHYDROXYDIPHENYLPROPANE	No	C15H16O2	228.291	680.90	360.50	1140.57	633.65
1491	1-N-PENTYLNAPHTHALENE	No	C15H18	198.308	582.80	306.00	1042.47	579.15
1491	1-PENTYLNAPHTHALENE	No	C15H18	198.308	582.80	306.00	1042.47	579.15
1491	Synonym2=AMYLNAPHTHALENE	No	C15H18	198.308	582.80	306.00	1042.47	579.15
1491	1-ALPHA-NAPHTHALENE	No	C15H18	198.308	582.80	306.00	1042.47	579.15
1492	N-NONYLBENZENE	No	C15H24	204.356	539.69	282.05	999.36	555.20
1492	NONYLBENZENE	No	C15H24	204.356	539.69	282.05	999.36	555.20
1492	1-PHENYLNONANE	No	C15H24	204.356	539.69	282.05	999.36	555.20
1493	NONYL PHENOL	No	C15H24O	220.355	603.70	317.61	1063.37	590.76
1494	FLUORANTHENE	No	C16H10	202.255	721.04	382.80	1180.71	655.95

1494	1,2-(1,8-NAPHTHYLENE)BENZENE	No	C16H10	202.255	721.04	382.80	1180.71	655.95
1494	1,2-BENZACENAPHTHENE	No	C16H10	202.255	721.04	382.80	1180.71	655.95
1494	IDRYLBENZO(JK)FLUORENE	No	C16H10	202.255	721.04	382.80	1180.71	655.95
1495	PYRENE	No	C16H10	202.255	742.64	394.80	1202.31	667.95
1495	BENZO(DEF)PHENANTHRENE	No	C16H10	202.255	742.64	394.80	1202.31	667.95
1496	N-DECYLBENZENE	No	C16H26	218.382	568.20	297.89	1027.87	571.04
1496	1-PHENYLDECANE	No	C16H26	218.382	568.20	297.89	1027.87	571.04
1496	DECYLBENZENE	No	C16H26	218.382	568.20	297.89	1027.87	571.04
1497	CHRYSENE	No	C18H12	228.293	825.80	441.00	1285.47	714.15
1497	1,2-BENZOPHENANTHRENE	No	C18H12	228.293	825.80	441.00	1285.47	714.15
1497	BENZO(A)PHENANTHRENE	No	C18H12	228.293	825.80	441.00	1285.47	714.15
1497	1,2-BENZPHENANTHRENE	No	C18H12	228.293	825.80	441.00	1285.47	714.15
1498	M-TERPHENYL	No	C18H14	230.309	707.00	375.00	1166.67	648.15
1498	1,3-DIPHENYLBENZENE	No	C18H14	230.309	707.00	375.00	1166.67	648.15
1498	ISODIPHENYLBENZENE	No	C18H14	230.309	707.00	375.00	1166.67	648.15
1498	3-PHENYLDIPHENYL	No	C18H14	230.309	707.00	375.00	1166.67	648.15
1498	3-PHENYLBIPHENYL	No	C18H14	230.309	707.00	375.00	1166.67	648.15
1499	O-TERPHENYL	No	C18H14	230.309	636.80	336.00	1096.47	609.15
1499	1,2-DIPHENYLBENZENE	No	C18H14	230.309	636.80	336.00	1096.47	609.15
1499	2-PHENYLDIPHENYL	No	C18H14	230.309	636.80	336.00	1096.47	609.15
1499	2-PHENYLBIPHENYL	No	C18H14	230.309	636.80	336.00	1096.47	609.15
1500	P-TERPHENYL	No	C18H14	230.309	719.60	382.00	1179.27	655.15
1500	1,4-DIPHENYLBENZENE	No	C18H14	230.309	719.60	382.00	1179.27	655.15
1500	P-DIPHENYLBENZENE	No	C18H14	230.309	719.60	382.00	1179.27	655.15
1500	4-PHENYLDIPHENYL	No	C18H14	230.309	719.60	382.00	1179.27	655.15
1500	4-PHENYLBIPHENYL	No	C18H14	230.309	719.60	382.00	1179.27	655.15
1501	2,3-DIMETHYL-2,3-DIPHENYLBUTANE	No	C18H22	238.373	600.53	315.85	1060.20	589.00
1501	1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)BISBENZENE	No	C18H23	239.373	602.33	316.85	1062.00	590.00
1501	DICUMYL	No	C18H24	240.373	604.13	317.85	1063.80	591.00
1501	TETRAMETHYL BIPHENYL ETHANE	No	C18H25	241.373	605.93	318.85	1065.60	592.00
1501	TETRAMETHYL BIBENZYL	No	C18H26	242.373	607.73	319.85	1067.40	593.00
1502	DIBUTYL SEBACATE	No	C18H34O4	314.466	660.20	349.00	1119.87	622.15
1502	DI-N-BUTYL SEBACATE	No	C18H34O4	314.466	660.20	349.00	1119.87	622.15
1502	BIS(N-BUTYL) SEBACATE	No	C18H34O4	314.466	660.20	349.00	1119.87	622.15
1502	DIBUTYL ESTER SEBACIC ACID	No	C18H34O4	314.466	660.20	349.00	1119.87	622.15
1502	DIBUTYL ESTER DECANEDIOIC ACID	No	C18H34O4	314.466	660.20	349.00	1119.87	622.15
1503	DIHEXYL ADIPATE	No	C18H34O4	314.466	658.40	348.00	1118.07	621.15
1503	DIHEXYL ESTER HEXANDIOIC ACID	No	C18H34O4	314.466	658.40	348.00	1118.07	621.15
1504	TRIPHENYLMETHANE	No	C19H16	244.336	678.20	359.00	1137.87	632.15
1504	TRITAN	No	C19H16	244.336	678.20	359.00	1137.87	632.15
1504	1,1',1''-METHYLIDYNETRISBENZENE	No	C19H16	244.336	678.20	359.00	1137.87	632.15
1504	1,1,1METHYLIDYNETRISBENZENE	No	C19H16	244.336	678.20	359.00	1137.87	632.15
1505	1-N-NONYLNAPHTHALENE	No	C19H26	254.415	690.53	365.85	1150.20	639.00
1506	1-NONADECENE	No	C19H38	266.511	624.24	329.02	1083.91	602.17
1507	TRIPHENYLETHYLENE	No	C20H16	256.347	744.53	395.85	1204.20	669.00
1507	1,1',1''-(1-ETHENYL-2-YLIDENE)TRISBENZENE	No	C20H16	256.347	744.53	395.85	1204.20	669.00
1508	1,1,2-TRIPHENYLETHANE	No	C20H18	258.363	659.93	348.85	1119.60	622.00
1508	1,1',1''-(1-ETHANYL-2-YLIDENE)TRISBENZENE	No	C20H18	258.363	659.93	348.85	1119.60	622.00
1509	1-N-DECYLNAPHTHALENE	No	C20H28	268.442	713.93	378.85	1173.60	652.00
1510	ABIETIC ACID	No	C20H30O2	302.457	709.79	376.55	1169.46	649.70
1510	SYLVIC ACID	No	C20H30O2	302.457	709.79	376.55	1169.46	649.70
1510	13-ISOPROPYLPODOCARPA-7,13-DIEN-15-OIC ACID	No	C20H30O2	302.457	709.79	376.55	1169.46	649.70
1511	N-TETRADECYLBENZENE	No	C20H34	274.49	669.20	354.00	1128.87	627.15
1511	1-PHENYLTETRADECANE	No	C20H34	274.49	669.20	354.00	1128.87	627.15
1511	TETRADECYLBENZENE	No	C20H34	274.49	669.20	354.00	1128.87	627.15
1512	EICOSENE	No	C20H40	280.538	648.30	342.39	1107.97	615.54
1512	1-EICOSENE	No	C20H40	280.538	648.30	342.39	1107.97	615.54
1513	N-PENTADECYLBENZENE	No	C21H36	288.517	690.80	366.00	1150.47	639.15
1513	PENTADECYLBENZENE	No	C21H36	288.517	690.80	366.00	1150.47	639.15
1513	1-PHENYL-PENTADECANE	No	C21H36	288.517	690.80	366.00	1150.47	639.15
1514	MONOOLEIN	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	(Z)-2,3-DIHYDROXYPROPYL ESTER 9-OCTADECENOIC ACID	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	GLYCEROL OLEATE	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	1-MONOOLEIN	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	ALPHA-MONOOLEIN	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	1-(9-OCTADECENOATE) GLYCEROL	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	ALPHA-MONOOLEATE	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00
1514	1-OLEATE GLYCEROL	No	C21H40O4	356.546	825.53	440.85	1285.20	714.00

## Chapter 2

1515	DIHEPTYL PHTHALATE	No	C22H34O4	362.51	733.73	389.85	1193.40	663.00
1515	DIHEPTYL ESTER 1,2-BENZENE DICARBOXYLIC ACID	No	C22H34O4	362.51	733.73	389.85	1193.40	663.00
1515	DIHEPTYL ESTER PHTHALIC ACID	No	C22H34O4	362.51	733.73	389.85	1193.40	663.00
1515	DI-N-HEPTYL PHTHALATE	No	C22H34O4	362.51	733.73	389.85	1193.40	663.00
1516	N-HEXADECYLBENZENE	No	C22H38	302.544	712.40	378.00	1172.07	651.15
1516	HEXADECYLBENZENE	No	C22H38	302.544	712.40	378.00	1172.07	651.15
1516	1-PHENYL-HEXADECANE	No	C22H38	302.544	712.40	378.00	1172.07	651.15
1517	DI-(2-ETHYLHEXYL)ADIPATE	No	C22H42O4	370.573	782.60	417.00	1242.27	690.15
1517	BIS(2-ETHYLHEXYL)ESTER HEXANEDIOIC ACID	No	C22H42O4	370.573	782.60	417.00	1242.27	690.15
1517	OCTYL ADIPATE	No	C22H42O4	370.573	782.60	417.00	1242.27	690.15
1518	DIOCTYL ADIPATE	No	C22H42O4	370.573	760.73	404.85	1220.40	678.00
1518	DIOCTYL ESTER HEXANEDIOIC ACID	No	C22H42O4	370.573	760.73	404.85	1220.40	678.00
1519	N-BUTYL STEARATE	No	C22H44O2	340.59	662.00	350.00	1121.67	623.15
1519	BUTYL ESTER OCTADECANOIC ACID	No	C22H44O2	340.59	662.00	350.00	1121.67	623.15
1519	BUTYL STEARATE	No	C22H44O2	340.59	662.00	350.00	1121.67	623.15
1520	N-HEPTADECYLBENZENE	No	C23H40	316.571	732.20	389.00	1191.87	662.15
1520	HEPTADECYLBENZENE	No	C23H40	316.571	732.20	389.00	1191.87	662.15
1520	1-PHENYLHEPTADECANE	No	C23H40	316.571	732.20	389.00	1191.87	662.15
1521	DIOCTYL PHTHALATE	No	C24H38O4	390.563	723.20	384.00	1182.87	657.15
1521	DOP	No	C24H38O4	390.563	723.20	384.00	1182.87	657.15
1521	OCTOIL	No	C24H38O4	390.563	723.20	384.00	1182.87	657.15
1521	BIS(2-ETHYLHEXYL) PHTHALATE	No	C24H38O4	390.563	723.20	384.00	1182.87	657.15
1521	DIOCTYL ESTER O-BENZENEDICARBOXYLIC ACID	No	C24H38O4	390.563	723.20	384.00	1182.87	657.15
1522	N-OCTADECYLBENZENE	No	C24H42	330.597	752.00	400.00	1211.67	673.15
1522	OCTADECYLBENZENE	No	C24H42	330.597	752.00	400.00	1211.67	673.15
1522	1-PHENYLOCTADECANE	No	C24H42	330.597	752.00	400.00	1211.67	673.15
1523	DINONYLPHENOL	No	C24H42O	346.597	863.33	461.85	1323.00	735.00
1523	2,4-DINONYLPHENOL	No	C24H42O	346.597	863.33	461.85	1323.00	735.00
1524	TRI-N-OCTYLAMINE	No	C24H51N	353.676	690.80	366.00	1150.47	639.15
1524	N,N-DIOCTYL-1-OCTANAMINE	No	C24H51N	353.676	690.80	366.00	1150.47	639.15
1524	TRIOCTYLAMINE	No	C24H51N	353.676	690.80	366.00	1150.47	639.15
1524	N,N-DIOCTYLOCTANAMINE	No	C24H51N	353.676	690.80	366.00	1150.47	639.15
1525	TETRAPHENYLMETHANE	No	C25H20	320.434	877.73	469.85	1337.40	743.00
1525	1,1',1",1'''-METHANETETRAYLTETRAKISBENZENE	No	C25H20	320.434	877.73	469.85	1337.40	743.00
1526	DINONYL PHTHALATE	No	C26H42O4	418.617	812.93	433.85	1272.60	707.00
1526	DI-N-NONYL PHTHALATE	No	C26H42O4	418.617	812.93	433.85	1272.60	707.00
1526	BISOFLEX91	No	C26H42O4	418.617	812.93	433.85	1272.60	707.00
1526	DINONYL-1,2-BENZENEDICARBOXYLATE	No	C26H42O4	418.617	812.93	433.85	1272.60	707.00
1526	DINONYL ESTER-1,2-BENZENEDICARBOXYLOIC ACID	No	C26H42O4	418.617	812.93	433.85	1272.60	707.00
1527	SQUALANE	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1527	COSBIOL	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1527	2,6,10,15,19,23-HEXAMETHYLTETRACOSANE	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1527	PERHYDROSQUALENE	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1527	DODECAHYDROSQUALENE	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1527	ROBANE	No	C30H62	422.822	836.33	446.85	1296.00	720.00
1528	IRON	No	Fe	55.845	5180.36	2860.20	5640.03	3133.35
1529	SULFOLANE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	1,1-DIOXIDE TERAHYDROTHIOPHENE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	DIOXOThIOLAN	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	DIHYDROBUTADIENE SULFONE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	THIOPANE DIOXIDE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	TETRAMETHYLENE SULFONE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1529	CYCLOTETRAMETHYLENE SULFONE	No	C4H8O2S	120.172	549.14	287.30	1008.81	560.45
1530	NITROGEN TRIOXIDE	No	NO3	62.0049				
1531	NITROGEN PENTOXIDE	No	N2O5	108.01				
1532	HELIUM-4	No	HE	4.003	-452.07	-268.93	7.60	4.22
1532	HELIUM	No	HE	4.003	-452.07	-268.93	7.60	4.22

## Component Database - ID From 2000 to 2999

The components ID numbers between 2000-2999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, critical temperature, critical pressure, and vapor pressure (as a function of temperature in range at least from 200 to 760 mmHg). For other properties see *Component Properties Estimation Methods*.

DESIGN II ID	Name	Mixed Amine	Formula	Molecular Weight	BP (F)	BP (C)	BP (R)	BP (K)
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## Database Components

2001	DIETHYL KETONE	No	C5H10O	86.13	215.06	101.70	674.73	374.85
2001	3-PENTANONE	No	C5H10O	86.13	215.06	101.70	674.73	374.85
2002	3-METHYL-2-BUTANONE	No	C5H10O	86.13	201.92	94.40	661.59	367.55
2002	METHYL ISOPROPYL KETONE	No	C5H10O	86.13	201.92	94.40	661.59	367.55
2003	METHYL ACETATE	No	C3H6O2	74.08	135.18	57.32	594.85	330.47
2003	METHYL ETHANOATE	No	C3H6O2	74.08	135.18	57.32	594.85	330.47
2004	N-PROPYL ACETATE	No	C5H10O2	102.13	214.79	101.55	674.46	374.70
2004	N-PROPYL ETHANOATE	No	C5H10O2	102.13	214.79	101.55	674.46	374.70
2005	METHYL PROPANOATE	No	C4H8O2	88.11	175.46	79.70	635.13	352.85
2005	METHYL PROPIONATE	No	C4H8O2	88.11	175.46	79.70	635.13	352.85
2006	ETHYL PROPANOATE	No	C5H10O2	102.13	210.38	99.10	670.05	372.25
2006	ETHYL PROPIONATE	No	C5H10O2	102.13	210.38	99.10	670.05	372.25
2007	METHYL BUTANOATE	No	C5H10O2	102.13	216.86	102.70	676.53	375.85
2007	METHYL BUTYRATE	No	C5H10O2	102.13	216.86	102.70	676.53	375.85
2008	METHYL ISOBUTYRATE	No	C5H10O2	102.13	198.14	92.30	657.81	365.45
2008	METHYL2-METHYLPROPANOATE	No	C5H10O2	102.13	198.14	92.30	657.81	365.45
2009	PERFLUORO-N-HEPTANE	No	C7F16	388.05	180.45	82.47	640.12	355.62
2010	METHYL ISOBUTYL KETONE	No	C6H12O	100.16	241.70	116.50	701.37	389.65
2010	4-METHYL-2-PENTANONE	No	C6H12O	100.16	241.70	116.50	701.37	389.65
2011	ANISOLE	No	C7H8O	108.14	311.99	155.55	771.66	428.70
2011	METHOXYBENZENE	No	C7H8O	108.14	311.99	155.55	771.66	428.70
2012	ETHOXYBENZENE	No	C8H10O	122.17	337.95	169.97	797.62	443.12
2012	PHENETOLE	No	C8H10O	122.17	337.95	169.97	797.62	443.12
2013	PERFLUORO-N-PENTANE	No	C5F12	288.04	84.54	29.19	544.21	302.34
2014	PERFLUOROCYCLOHEXANE	No	C6F12	300.05	127.13	52.85	586.80	326.00
2015	PERFLUOROMETHYLCYCLOHEXANE	No	C7F14	350.06	169.34	76.30	629.01	349.45
2016	2-METHYLANILINE	No	C7H9N	107.16	391.55	199.75	851.22	472.90
2016	2-TOLUIDINE	No	C7H9N	107.16	391.55	199.75	851.22	472.90
2016	O-TOLUIDINE	No	C7H9N	107.16	391.55	199.75	851.22	472.90
2017	3-METHYLANILINE	No	C7H9N	107.16	398.03	203.35	857.70	476.50
2017	3-TOLUIDINE	No	C7H9N	107.16	398.03	203.35	857.70	476.50
2017	M-TOLUIDINE	No	C7H9N	107.16	398.03	203.35	857.70	476.50
2018	4-METHYLANILINE	No	C7H9N	107.16	392.81	200.45	852.48	473.60
2018	4-TOLUIDINE	No	C7H9N	107.16	392.81	200.45	852.48	473.60
2018	P-TOLUIDINE	No	C7H9N	107.16	392.81	200.45	852.48	473.60
2019	N-METHYLANILINE	No	C7H9N	107.16	383.99	195.55	843.66	468.70
2020	N-N-DIMETHYLANILINE	No	C8H11N	121.18	379.67	193.15	839.34	466.30
2020	DIMETHYL PHENYL AMINE	No	C8H11N	121.18	379.67	193.15	839.34	466.30
2021	N-N-DIMETHYL-O-TOLUIDINE	No	C9H13N	135.21	364.73	184.85	824.40	458.00
2022	BENZALDEHYDE	No	C7H6O	106.12	354.29	179.05	813.96	452.20
2023	ISOAMYL FORMATE	No	C6H12O2	116.16	253.76	123.20	713.43	396.35
2023	ISOPENTYL FORMATE	No	C6H12O2	116.16	253.76	123.20	713.43	396.35
2023	ISOPENTYL METHANOATE	No	C6H12O2	116.16	253.76	123.20	713.43	396.35
2024	ISOBUTYL ACETATE	No	C6H12O2	116.16	242.78	117.10	702.45	390.25
2024	ISOBUTYL ETHANOATE	No	C6H12O2	116.16	242.78	117.10	702.45	390.25
2025	ETHYL BUTANOATE	No	C6H12O2	116.16	250.79	121.55	710.46	394.70
2025	ETHYL BUTYRATE	No	C6H12O2	116.16	250.79	121.55	710.46	394.70
2026	FLUOROETHENE	No	C2FH3	46.04	-97.87	-72.15	361.80	201.00
2026	VINYL FLUORIDE	No	C2FH3	46.04	-97.87	-72.15	361.80	201.00
2026	REFRIGERANT 1141	No	C2FH3	46.04	-97.87	-72.15	361.80	201.00
2026	R1141	No	C2FH3	46.04	-97.87	-72.15	361.80	201.00
2026	R-1141	No	C2FH3	46.04	-97.87	-72.15	361.80	201.00
2027	ISOAMYL ACETATE	No	C7H14O2	130.19	283.64	139.80	743.31	412.95
2027	ISOPENTYL ETHANOATE	No	C7H14O2	130.19	283.64	139.80	743.31	412.95
2028	N-PROPYL PROPANOATE	No	C6H12O2	116.16	253.76	123.20	713.43	396.35
2028	N-PROPYL PROPIONATE	No	C6H12O2	116.16	253.76	123.20	713.43	396.35
2029	2,6-DIMETHYL PYRIDINE	No	C7H9N	107.16	291.28	144.04	750.95	417.19
2029	2,6-LUTIDINE	No	C7H9N	107.16	291.28	144.04	750.95	417.19
2030	PIPERIDINE	No	C5H11N	85.15	222.89	106.05	682.56	379.20
2031	N-BUTYL ACETATE	No	C6H12O2	116.16	258.99	126.11	718.66	399.26
2031	N-BUTYL ETHANOATE	No	C6H12O2	116.16	258.99	126.11	718.66	399.26
2032	ISOAMYL PROPIONATE	No	C8H16O2	144.22	321.08	160.60	780.75	433.75
2032	ISOPENTYL PROPANOATE	No	C8H16O2	144.22	321.08	160.60	780.75	433.75
2032	ISOPENTYL PROPIONATE	No	C8H16O2	144.22	321.08	160.60	780.75	433.75
2033	ETHYL PENTANOATE	No	C7H14O2	130.19	293.18	145.10	752.85	418.25
2033	ETHYL VALERATE	No	C7H14O2	130.19	293.18	145.10	752.85	418.25
2034	ETHYL-N-CAPRYLATE	No	C10H20O2	172.27	407.30	208.50	866.97	481.65
2034	ETHYL OCTANOATE	No	C10H20O2	172.27	407.30	208.50	866.97	481.65
2035	ETHYL NONANOATE	No	C11H22O2	186.30	440.63	227.02	900.30	500.17
2035	ETHYL NONYLATE	No	C11H22O2	186.30	440.63	227.02	900.30	500.17
2035	ETHYL-N-PELARGONATE	No	C11H22O2	186.30	440.63	227.02	900.30	500.17

## Chapter 2

2036	PERFLUORONAPHTHALENE	No	C10F8	272.10	284.00	140.00	743.67	413.15
2037	DIMETHYL OXALATE	No	C4H6O4	118.09	326.03	163.35	785.70	436.50
2038	ISOBUTYL ALCOHOL	No	C4H10O	74.12	225.79	107.66	685.46	380.81
2038	2-METHYL-1-PROPANOL	No	C4H10O	74.12	225.79	107.66	685.46	380.81
2039	ISOBUTYLBENZENE	No	C10H14	134.22	343.02	172.79	802.69	445.94
2039	1-PHENYL-2-METHYLPROPANE	No	C10H14	134.22	343.02	172.79	802.69	445.94
2040	PROPANOIC ACID	No	C3H6O2	74.08	285.49	140.83	745.16	413.98
2040	PROPIONIC ACID	No	C3H6O2	74.08	285.49	140.83	745.16	413.98
2041	BUTANOIC ACID	No	C4H8O2	88.10	325.89	163.27	785.56	436.42
2041	BUTYRIC ACID	No	C4H8O2	88.10	325.89	163.27	785.56	436.42
2042	TETRAHYDROFURAN	No	C4H8O	72.10	150.73	65.96	610.40	339.11
2042	TETRAMETHYLENE OXIDE	No	C4H8O	72.10	150.73	65.96	610.40	339.11
2043	(2-PENTYL)-BENZENE	No	C11H16	148.25	379.43	193.02	839.10	466.17
2043	2-PHENYLPENTANE	No	C11H16	148.25	379.43	193.02	839.10	466.17
2044	2,3-DIMETHYL-1-ETHYLBENZENE	No	C10H14	134.22	381.13	193.96	840.80	467.11
2044	3-ETHYL-O-XYLENE	No	C10H14	134.22	381.13	193.96	840.80	467.11
2045	1,3-DIMETHYL-2-ETHYLBENZENE	No	C10H14	134.22	374.07	190.04	833.74	463.19
2045	2-ETHYL-M-XYLENE	No	C10H14	134.22	374.07	190.04	833.74	463.19
2046	1,2-DIETHYL-3-METHYLBENZENE	No	C11H16	148.25	403.93	206.63	863.60	479.78
2046	2,3-DIETHYLTOLUENE	No	C11H16	148.25	403.93	206.63	863.60	479.78
2047	1,3-DIETHYL-2-METHYLBENZENE	No	C11H16	148.25	407.83	208.79	867.50	481.94
2047	2,6-DIETHYLTOLUENE	No	C11H16	148.25	407.83	208.79	867.50	481.94
2048	ETHYL FORMATE	No	C3H6O2	74.08	129.54	54.19	589.21	327.34
2048	ETHYL METHANOATE	No	C3H6O2	74.08	129.54	54.19	589.21	327.34
2049	ISOBUTYRIC ACID	No	C4H8O2	88.11	310.28	154.60	769.95	427.75
2049	2-METHYLPROPANOIC ACID	No	C4H8O2	88.11	310.28	154.60	769.95	427.75
2050	N-PROPYL FORMATE	No	C4H8O2	88.11	177.53	80.85	637.20	354.00
2050	N-PROPYL METHANOATE	No	C4H8O2	88.11	177.53	80.85	637.20	354.00
2051	ISOBUTYL FORMATE	No	C5H10O2	102.13	208.53	98.07	668.20	371.22
2051	ISOBUTYL METHANOATE	No	C5H10O2	102.13	208.53	98.07	668.20	371.22
2052	ETHYL PROPYL ETHER	No	C5H12O	88.15	146.95	63.86	606.62	337.01
2053	DIGLYCOLAMINE	Yes	C4H11NO2	105.14	430.00	221.11	889.67	494.26
2053	DGA	Yes	C4H11NO2	105.14	430.00	221.11	889.67	494.26
2054	THERMINOL 66	No		252.00	678.00	359.00	1137.67	632.15
2055	THERMINOL 55	No		320.00	664.00	351.00	1123.70	624.15
2056	THERMINOL 72	No		190.00	520.00	271.11	979.67	544.26
2057	THERMINOL 75	No		230.00	649.00	342.78	1108.67	615.93
2058	THERMINOL VP-1	No		166.00	495.00	257.00	800.20	444.56
2058	DOWTHERM A	No		166.00	495.00	257.00	800.20	444.56
2059	CHEMTHERM 550®	No		350.00	524.00	273.33	983.67	546.48
2060	R245fa	No	C3H3F5	134.05	58.82	14.90	288.05	518.49
2060	Genetron® 245fa	No	C3H3F5	134.05	58.82	14.90	288.05	518.49
2060	1,1,1,3,3-Pentafluoropropane	No	C3H3F5	134.05	58.82	14.90	288.05	518.49
2060	Refrigerant 245fa	No	C3H3F5	134.05	58.82	14.90	288.05	518.49
2060	R-245fa	No	C3H3F5	134.05	58.82	14.90	288.05	518.49
2061	THERMINOL 59	No		207.00	553.00	289.44	1012.67	562.59

## Component Database - ID From 3000 to 3999

The components ID numbers between 3000-3999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, heat capacity, and vapor pressure (as a function of temperature in range at least from 200 to 760 mmHg). For other properties see *Component Properties Estimation Methods*.

DESIGN II ID	Name	Mixed Amine	Molecular Formula	Molecular Weight	BP (F)	BP (C)	BP (R)	BP (K)
3001	3,4-DI-THIAHEXANE	No	C4H10S2	122.25	309.16	153.98	768.83	427.13
3001	ETHYL DISULFIDE	No	C4H10S2	122.25	309.16	153.98	768.83	427.13
3002	2-METHYL PYRIDINE	No	C6H7N	93.13	264.90	129.39	724.57	402.54
3002	2-PICOLINE	No	C6H7N	93.13	264.90	129.39	724.57	402.54
3003	TETRAHYDROTHIOPHENE	No	C4H8S	88.17	250.01	121.12	709.68	394.27
3003	TETRAMETHYLENE SULFIDE	No	C4H8S	88.17	250.01	121.12	709.68	394.27
3003	THIACYCLOPENTANE	No	C4H8S	88.17	250.01	121.12	709.68	394.27
3004	AMYL ALCOHOL	No	C5H12O	88.15	280.40	138.00	740.07	411.15
3004	PENTYL ALCOHOL	No	C5H12O	88.15	280.40	138.00	740.07	411.15
3005	T-AMYL ALCOHOL	No	C5H12O	88.15	216.23	102.35	675.90	375.50
3005	2-METHYL-2-BUTANOL	No	C5H12O	88.15	216.23	102.35	675.90	375.50
3005	T-PENTYL ALCOHOL	No	C5H12O	88.15	216.23	102.35	675.90	375.50
3006	1-HEXANOL	No	C6H14O	102.17	314.60	157.00	774.27	430.15
3006	HEXYL ALCOHOL	No	C6H14O	102.17	314.60	157.00	774.27	430.15
3007	1-NONANOL	No	C9H20O	144.25	416.30	213.50	875.97	486.65



# Database Components

3007	NONYL ALCOHOL	No	C9H20O	144.25	416.30	213.50	875.97	486.65
3008	1-DECANOL	No	C10H22O	158.27	446.09	230.05	905.76	503.20
3008	DECYL ALCOHOL	No	C10H22O	158.27	446.09	230.05	905.76	503.20
3009	SEC-BUTYL CHLORIDE	No	C4H9CL	92.57	154.85	68.25	614.52	341.40
3009	2-CHLOROBUTANE	No	C4H9CL	92.57	154.85	68.25	614.52	341.40
3010	CYANOGEN BROMIDE	No	CBRN	105.93	142.70	61.50	602.37	334.65
3011	CYANOGEN CHLORIDE	No	CCLN	61.47	55.58	13.10	515.25	286.25
3012	CARBON SUBOXIDE	No	C3O2	68.03	43.52	6.40	503.19	279.55
3013	NITRYL CHLORIDE	No	CLNO2	81.46	4.46	-15.30	464.13	257.85
3014	THIONYL CHLORIDE	No	SOCL2	118.98	168.35	75.75	628.02	348.90
3015	SULFURYL CHLORIDE	No	SO2CL2	134.98	156.65	69.25	616.32	342.40
3016	SULFUR MONOCHLORIDE	No	S2CL2	135.04	279.68	137.60	739.35	410.75
3017	HYDROGEN NITRATE	No	HNO3	63.02	181.40	83.00	641.07	356.15
3017	NITRIC ACID	No	HNO3	63.02	181.40	83.00	641.07	356.15
3018	HYDROGEN PEROXIDE	No	H2O2	34.02	302.36	150.20	762.03	423.35
3019	UNDECYL ALCOHOL	No	C11H24O	172.30	473.00	245.00	932.67	518.15
3020	DODECYL ALCOHOL	No	C12H26O	186.32	500.00	260.00	959.67	533.15
3021	1-TRIDECANOL	No	C13H28O	200.35	525.20	274.00	984.87	547.15
3022	1-TETRADECANOL	No	C14H30O	214.38	548.60	287.00	1008.27	560.15
3023	1-PENTADECANOL	No	C15H32O	228.40	572.00	300.00	1031.67	573.15
3024	CETYL ALCOHOL	No	C16H34O	242.43	593.60	312.00	1053.27	585.15
3024	1-HEXADECANOL	No	C16H34O	242.43	593.60	312.00	1053.27	585.15
3025	1-HEPTADECANOL	No	C17H36O	256.45	615.13	323.96	1074.80	597.11
3026	1-OCTADECANOL	No	C18H38O	270.48	635.00	335.00	1094.67	608.15
3027	1-NONADECANOL	No	C19H40O	284.51	653.00	345.00	1112.67	618.15
3028	EICOSANOL	No	C20H42O	298.53	672.80	356.00	1132.47	629.15
3028	METHANOIC ACID	No	C20H42O	298.53	672.80	356.00	1132.47	629.15
3029	FORMALDEHYDE	No	CH2O	30.03	-2.65	-19.25	457.02	253.90
3029	METHANAL	No	CH2O	30.03	-2.65	-19.25	457.02	253.90
3030	PROPIONALDEHYDE	No	C3H6O	58.08	118.13	47.85	577.80	321.00
3031	BUTYRALDEHYDE	No	C4H8O	72.10	166.73	74.85	626.40	348.00
3031	1-BUTANAL	No	C4H8O	72.10	166.73	74.85	626.40	348.00
3032	PENTANAL	No	C5H10O	86.13	216.59	102.55	676.26	375.70
3032	VALERALDEHYDE	No	C5H10O	86.13	216.59	102.55	676.26	375.70
3033	HEXANAL	No	C6H12O	100.15	263.75	128.75	723.42	401.90
3034	ENANTHALDEHYDE	No	C7H14O	114.18	306.77	152.65	766.44	425.80
3034	HEPTALDEHYDE	No	C7H14O	114.18	306.77	152.65	766.44	425.80
3034	HEPTANAL	No	C7H14O	114.18	306.77	152.65	766.44	425.80
3035	CAPRYALDEHYDE	No	C8H16O	128.20	343.13	172.85	802.80	446.00
3035	OCTANAL	No	C8H16O	128.20	343.13	172.85	802.80	446.00
3036	NONANAL	No	C9H18O	142.23	380.93	193.85	840.60	467.00
3036	PELARGONIC ALDEHYDE	No	C9H18O	142.23	380.93	193.85	840.60	467.00
3037	CAPRALDEHYDE	No	C10H20O	156.26	415.13	212.85	874.80	486.00
3037	DECANAL	No	C10H20O	156.26	415.13	212.85	874.80	486.00
3038	FORMIC ACID	No	CH2O2	46.03	212.99	100.55	672.66	373.70
3039	ACRYLIC ACID	No	C3H4O2	72.06	285.89	141.05	745.56	414.20
3039	PROPENOIC ACID	No	C3H4O2	72.06	285.89	141.05	745.56	414.20
3040	BENZOIC ACID	No	C7H6O2	122.11	480.65	249.25	940.32	522.40
3041	ACRYLONITRILE	No	C3H3N	53.06	171.23	77.35	630.90	350.50
3041	2-PROPENENITRILE	No	C3H3N	53.06	171.23	77.35	630.90	350.50
3042	NITROETHANE	No	C2H5NO2	75.07	237.32	114.07	696.99	387.22
3043	1-NITROPROPANE	No	C3H7NO2	89.09	268.12	131.18	727.79	404.33
3044	2-NITROPROPANE	No	C3H7NO2	89.09	248.45	120.25	708.12	393.40
3045	1-NITROBUTANE	No	C4H9NO2	103.12	306.98	152.77	766.65	425.92
3046	2-NITROBUTANE	No	C4H9NO2	103.12	283.10	139.50	742.77	412.65
3047	DIFLUOROMETHANE	No	CH2F2	52.03	-60.88	-51.60	398.79	221.55
3047	METHYLENE FLUORIDE	No	CH2F2	52.03	-60.88	-51.60	398.79	221.55
3047	REFRIGERANT 32	No	CH2F2	52.03	-60.88	-51.60	398.79	221.55
3047	R32	No	CH2F2	52.03	-60.88	-51.60	398.79	221.55
3047	R-32	No	CH2F2	52.03	-60.88	-51.60	398.79	221.55
3048	1-FLUOROPROPANE	No	C3H7F	62.09	27.59	-2.45	487.26	270.70
3049	PHENYL-CF3	No	C7H5F3	146.11	215.69	102.05	675.36	375.20
3049	BENZOTRIFLUORIDE	No	C7H5F3	146.11	215.69	102.05	675.36	375.20
3049	$\alpha$ -TRIFLUOROTOLUENE	No	C7H5F3	146.11	215.69	102.05	675.36	375.20
3050	CL2HC-CH2CL	No	C2H3CL3	133.41	237.29	114.05	696.96	387.20
3050	1,1,2-TRICHLOROETHANE	No	C2H3CL3	133.41	237.29	114.05	696.96	387.20
3051	HCL2C-CCL2H	No	C2H2CL4	167.86	295.23	146.24	754.90	419.39
3051	1,1,2,2-TETRACHLOROETHANE	No	C2H2CL4	167.86	295.23	146.24	754.90	419.39
3052	PENTACHLOROETHANE	No	C2HCL5	202.31	318.83	159.35	778.50	432.50
3052	REFRIGERANT 120	No	C2HCL5	202.31	318.83	159.35	778.50	432.50
3052	R120	No	C2HCL5	202.31	318.83	159.35	778.50	432.50

## Chapter 2

3052	R-120	No	C2HCL5	202.31	318.83	159.35	778.50	432.50
3053	2-CHLOROPROPANE	No	C3H7CL	78.54	94.73	34.85	554.40	308.00
3054	1,2-DICHLOROPROPANE	No	C3H6CL2	112.99	205.46	96.37	665.13	369.52
3055	1,2,3-TRICHLOROPROPANE	No	C3H5CL3	147.44	314.33	156.85	774.00	430.00
3056	1-CHLORO-2-METHYL PROPANE	No	C4H9CL	92.57	155.93	68.85	615.60	342.00
3056	ISOBUTYL CHLORIDE	No	C4H9CL	92.57	155.93	68.85	615.60	342.00
3057	T-BUTYL CHLORIDE	No	C4H9CL	92.57	123.35	50.75	583.02	323.90
3057	2-CHLORO-2-METHYL PROPANE	No	C4H9CL	92.57	123.35	50.75	583.02	323.90
3058	TETRACHLOROETHENE	No	C2CL4	165.84	249.89	121.05	709.56	394.20
3058	TETRACHLOROETHYLENE	No	C2CL4	165.84	249.89	121.05	709.56	394.20
3059	1,4-DICHLOROBENZENE	No	C6H4CL2	147.00	345.30	174.06	804.97	447.21
3059	P-DICHLOROBENZENE	No	C6H4CL2	147.00	345.30	174.06	804.97	447.21
3060	2-BROMOPROPANE	No	C3H7BR	123.00	138.93	59.41	598.60	332.56
3061	1,2-DIBROMOPROPANE	No	C3H6BR2	201.91	284.99	140.55	744.66	413.70
3062	2-BROMO-2-METHYL PROPANE	No	C4H9BR	137.02	163.49	73.05	623.16	346.20
3062	T-BUTYL BROMIDE	No	C4H9BR	137.02	163.49	73.05	623.16	346.20
3063	1,2-DIBROMOBUTANE	No	C4H8BR2	215.93	331.43	166.35	791.10	439.50
3064	2,3-DIBROMOBUTANE	No	C4H8BR2	215.93	320.99	160.55	780.66	433.70
3065	BROMOETHENE	No	C4H8BR2	106.96	60.44	15.80	520.11	288.95
3065	BROMOETHYLENE	No	C4H8BR2	106.96	60.44	15.80	520.11	288.95
3065	VINYL BROMIDE	No	C4H8BR2	106.96	60.44	15.80	520.11	288.95
3066	DIIODOMETHANE	No	CH2I2	267.84	359.33	181.85	819.00	455.00
3066	METHYLENE IODIDE	No	CH2I2	267.84	359.33	181.85	819.00	455.00
3067	2-IODOPROPANE	No	C3H7I	169.99	193.01	89.45	652.68	362.60
3068	ISOPROPYLMETHYLSULFIDE	No	C4H10S	90.19	184.67	84.82	644.34	357.97
3069	METHYLPROPYLSULFIDE	No	C4H10S	90.19	203.97	95.54	663.64	368.69
3070	BUTYLMETHYLSULFIDE	No	C5H12S	104.21	254.15	123.42	713.82	396.57
3071	ETHYLMETHYLSULFIDE	No	C5H12S	104.21	245.30	118.50	704.97	391.65
3072	BUTYLETHYLSULFIDE	No	C6H14S	118.23	291.65	144.25	751.32	417.40
3073	ISOPROPYLSULFIDE	No	C6H14S	118.23	248.05	120.03	707.72	393.18
3074	PROPYLSULFIDE	No	C6H14S	118.23	289.11	142.84	748.78	415.99
3075	2,3-DI-THIABUTANE	No	C2H6S2	94.20	229.53	109.74	689.20	382.89
3075	METHYL DISULFIDE	No	C2H6S2	94.20	229.53	109.74	689.20	382.89
3076	PROPYL DISULFIDE	No	C6H14S2	150.30	384.54	195.86	844.21	469.01
3077	THIACYCLOPROPANE	No	C2H4S	60.12	130.83	54.91	590.50	328.06
3078	THIACYCLOBUTANE	No	C3H6S	74.14	202.93	94.96	662.60	368.11
3079	THIACYCLOHEXANE	No	C5H10S	102.19	287.15	141.75	746.82	414.90
3080	2-METHYLTHIOPHENE	No	C5H6S	98.16	234.60	112.56	694.27	385.71
3081	3-METHYLTHIOPHENE	No	C5H6S	98.16	239.79	115.44	699.46	388.59
3082	2-PROPANETHIOL	No	C3H8S	76.16	126.60	52.56	586.27	325.71
3083	2-BUTANETHIOL	No	C4H10S	90.19	184.96	84.98	644.63	358.13
3083	SEC-BUTYL MERCAPTAN	No	C4H10S	90.19	184.96	84.98	644.63	358.13
3084	2-METHYL-1-PROPANETHIOL	No	C4H10S	90.19	191.28	88.49	650.95	361.64
3084	ISOBUTYL MERCAPTAN	No	C4H10S	90.19	191.28	88.49	650.95	361.64
3085	T-BUTYL THIOL	No	C4H10S	90.19	147.59	64.22	607.26	337.37
3085	2-METHYL-2-PROPANETHIOL	No	C4H10S	90.19	147.59	64.22	607.26	337.37
3085	TERT-BUTYL MERCAPTAN	No	C4H10S	90.19	147.59	64.22	607.26	337.37
3086	2-METHYL-2-BUTANETHIOL	No	C5H12S	104.21	210.43	99.13	670.10	372.28
3086	TERT-AMYL MERCAPTAN	No	C5H12S	104.21	210.43	99.13	670.10	372.28
3087	1-HEXANETHIOL	No	C6H14S	118.23	306.68	152.60	766.35	425.75
3088	1-HEPTANETHIOL	No	C7H16S	132.26	349.25	176.25	808.92	449.40
3089	1-OCTANETHIOL	No	C8H18S	146.29	390.29	199.05	849.96	472.20
3090	1-NONANETHIOL	No	C9H20S	160.31	428.45	220.25	888.12	493.40
3091	1-DECANETHIOL	No	C10H22S	174.34	465.17	240.65	924.84	513.80
3092	1-UNDECANETHIOL	No	C11H24S	188.36	495.32	257.40	954.99	530.55
3093	1-DODECANETHIOL	No	C12H26S	202.39	526.28	274.60	985.95	547.75
3094	1-TRIDECANETHIOL	No	C13H28S	216.42	555.44	290.80	1015.11	563.95
3095	1-TETRADECANETHIOL	No	C14H30S	230.44	583.16	306.20	1042.83	579.35
3096	1-PENTADECANETHIOL	No	C15H32S	244.47	609.26	320.70	1068.93	593.85
3097	1-HEXADECANETHIOL	No	C16H34S	258.49	633.20	334.00	1092.87	607.15
3098	1-HEPTADECANETHIOL	No	C17H36S	272.52	658.40	348.00	1118.07	621.15
3099	1-OCTADECANETHIOL	No	C18H38S	286.55	680.00	360.00	1139.67	633.15
3100	1-NONADECANETHIOL	No	C19H40S	300.57	701.60	372.00	1161.27	645.15
3101	1-EICOSANETHIOL	No	C20H42S	314.60	721.40	383.00	1181.07	656.15
3102	BENZENETHIOL	No	C6H6S	110.17	336.45	169.14	796.12	442.29
3102	THIOPHENOL	No	C6H6S	110.17	336.45	169.14	796.12	442.29
3102	PHENYL MERCAPTAN	No	C6H6S	110.17	336.45	169.14	796.12	442.29
3103	1,2-ETHANEDIOL	No	C2H6O2	62.07	386.96	197.20	846.63	470.35
3103	ETHYLENE GLYCOL	No	C2H6O2	62.07	386.96	197.20	846.63	470.35
3103	EG	No	C2H6O2	62.07	386.96	197.20	846.63	470.35
3103	DIHYDROXY ETHANE	No	C2H6O2	62.07	386.96	197.20	846.63	470.35

# Database Components

3104	4-FLUOROTOLUENE	No	C7H7F	110.12	241.95	116.64	701.62	389.79
3104	P-FLUOROTOLUENE	No	C7H7F	110.12	241.95	116.64	701.62	389.79
3105	HEXACHLOROETHANE	No	C2CL6	236.76	363.92	184.40	823.59	457.55
3105	PERCHLOROETHANE	No	C2CL6	236.76	363.92	184.40	823.59	457.55
3106	1,1-DICHLOROETHENE	No	C2H2CL2	96.95	88.81	31.56	548.48	304.71
3106	1,1-DICHLOROETHYLENE	No	C2H2CL2	96.95	88.81	31.56	548.48	304.71
3106	VINYLDENE CHLORIDE	No	C2H2CL2	96.95	88.81	31.56	548.48	304.71
3107	1,3-DICHLOROBENZENE	No	C6H4CL2	147.00	343.53	173.07	803.20	446.22
3107	M-DICHLOROBENZENE	No	C6H4CL2	147.00	343.53	173.07	803.20	446.22
3108	BUTYL DISULFIDE	No	C8H18S2	178.35	448.13	231.18	907.80	504.33
3109	N-AMYLDISULFIDE	No	C10H22S2	206.40	507.02	263.90	966.69	537.05
3109	PENTYL DISULFIDE	No	C10H22S2	206.40	507.02	263.90	966.69	537.05
3110	ISOPROPENYL BENZENE	No	C9H10	118.18	329.72	165.40	789.39	438.55
3110	$\alpha$ METHYL STYRENE	No	C9H10	118.18	329.72	165.40	789.39	438.55
3111	METHYL CHLOROFORM	No	C2H3CL3	133.41	165.38	74.10	625.05	347.25
3111	1,1,1-TRICHLOROETHANE	No	C2H3CL3	133.41	165.38	74.10	625.05	347.25
3112	2 BUTOXYETHANOL	No	C6H14O2	118.18	339.80	171.00	799.47	444.15
3112	ETHYLENE GLYCOL MONOBUTYL ETHER	No	C6H14O2	118.18	339.80	171.00	799.47	444.15
3113	2 ETHOXYETHANOL	No	C4H10O2	90.12	275.00	135.00	734.67	408.15
3113	ETHYLENE GLYCOL MONOETHYL ETHER	No	C4H10O2	90.12	275.00	135.00	734.67	408.15
3114	2-BUTYNE	No	C4H6	54.09	80.55	26.97	540.22	300.12
3114	DIMETHYLACETYLENE	No	C4H6	54.09	80.55	26.97	540.22	300.12
3115	CYCLOBUTANE	No	C4H8	56.10	54.52	12.51	514.19	285.66
3116	CYCLOBUTENE	No	C4H6	54.09	36.41	2.45	496.08	275.60
3117	2-ETHYL-1-BUTENE	No	C6H12	84.16	148.43	64.68	608.10	337.83
3117	2-METHYLENEPENTANE	No	C6H12	84.16	148.43	64.68	608.10	337.83
3118	CIS-2-HEXENE	No	C6H12	84.16	156.00	68.89	615.67	342.04
3119	TRANS-2-HEXENE	No	C6H12	84.16	154.19	67.88	613.86	341.03
3120	CIS-3-HEXENE	No	C6H12	84.16	151.61	66.45	611.28	339.60
3121	TRANS-3-HEXENE	No	C6H12	84.16	152.76	67.09	612.43	340.24
3122	ISOPRENE	No	C5H8	68.11	93.31	34.06	552.98	307.21
3122	2-METHYL-1,3-BUTADIENE	No	C5H8	68.11	93.31	34.06	552.98	307.21
3123	ASYM-DIMETHYLLALLENE	No	C5H8	68.11	105.49	40.83	565.16	313.98
3123	3-METHYL-1,2-BUTADIENE	No	C5H8	68.11	105.49	40.83	565.16	313.98
3124	2-METHYL-1-PENTENE	No	C6H12	84.16	143.80	62.11	603.47	335.26
3125	2-METHYL-2-PENTENE	No	C6H12	84.16	153.15	67.31	612.82	340.46
3126	3-METHYL-1-PENTENE	No	C6H12	84.16	129.52	54.18	589.19	327.33
3127	3-METHYL-CIS-2-PENTENE	No	C6H12	84.16	153.86	67.70	613.53	340.85
3128	3-METHYL-TRANS-2-PENTENE	No	C6H12	84.16	158.79	70.44	618.46	343.59
3129	4-METHYL-1-PENTENE	No	C6H12	84.16	128.96	53.87	588.63	327.02
3130	4-METHYL-CIS-2-PENTENE	No	C6H12	84.16	133.50	56.39	593.17	329.54
3131	4-METHYL-TRANS-2-PENTENE	No	C6H12	84.16	137.50	58.61	597.17	331.76
3132	ETHYLLALLENE	No	C5H8	68.11	112.73	44.85	572.40	318.00
3132	1,2-PENTADIENE	No	C5H8	68.11	112.73	44.85	572.40	318.00
3133	1,CIS-3-PENTADIENE	No	C5H8	68.11	111.30	44.06	570.97	317.21
3133	CIS-PIPERYLENE	No	C5H8	68.11	111.30	44.06	570.97	317.21
3134	1,TRANS-3-PENTADIENE	No	C5H8	68.11	107.64	42.02	567.31	315.17
3134	TRANS-PIPERYLENE	No	C5H8	68.11	107.64	42.02	567.31	315.17
3135	DIVINYLMETHANE	No	C5H8	68.11	78.72	25.96	538.39	299.11
3135	1,4-PENTADIENE	No	C5H8	68.11	78.72	25.96	538.39	299.11
3136	DIMETHYLLALLENE	No	C5H8	68.11	118.86	48.26	578.53	321.41
3136	2,3-PENTADIENE	No	C5H8	68.11	118.86	48.26	578.53	321.41
3137	1-PENTYNE	No	C5H8	68.11	104.31	40.17	563.98	313.32
3137	PROPYLACETYLENE	No	C5H8	68.11	104.31	40.17	563.98	313.32
3138	METHYL ETHYLACETYLENE	No	C5H8	68.11	132.91	56.06	592.58	329.21
3138	2-PENTYNE	No	C5H8	68.11	132.91	56.06	592.58	329.21
3139	CIS-BICYCLO 4.4.0 DECANE	No	C10H18	138.26	384.39	195.77	844.06	468.92
3139	CIS-DECAHYDRONAPHTHALENE	No	C10H18	138.26	384.39	195.77	844.06	468.92
3139	CIS-DECALIN	No	C10H18	138.26	384.39	195.77	844.06	468.92
3140	TRANS-BICYCLO 4.4.0 DECANE	No	C10H18	138.26	369.09	187.27	828.76	460.42
3140	TRANS-DECAHYDRONAPHTHALENE	No	C10H18	138.26	369.09	187.27	828.76	460.42
3140	TRANS-DECALIN	No	C10H18	138.26	369.09	187.27	828.76	460.42
3141	1-DECENE	No	C10H20	140.27	339.03	170.57	798.70	443.72
3141	$\alpha$ -DECYLENE	No	C10H20	140.27	339.03	170.57	798.70	443.72
3142	1,3-DIETHYLBENZENE	No	C10H14	134.22	358.05	181.14	817.72	454.29
3142	M-DIETHYLBENZENE	No	C10H14	134.22	358.05	181.14	817.72	454.29
3143	1-DODECENE	No	C12H24	168.32	416.04	213.36	875.71	486.51
3144	DODECYLBENZENE	No	C18H30	246.44	621.68	327.60	1081.35	600.75
3145	1-NONENE	No	C9H18	126.23	296.36	146.87	756.03	420.02
3146	1-TETRADECENE	No	C14H28	196.38	483.80	251.00	943.47	524.15
3147	1,2,3,4-TETRAHYDRONAPHTHALENE	No	C10H12	132.21	405.77	207.65	865.44	480.80

## Chapter 2

3147	TETRALIN	No	C10H12	132.21	405.77	207.65	865.44	480.80
3148	1-PHENYLTRIDECANE	No	C19H32	260.47	646.16	341.20	1105.83	614.35
3148	TRIDECYL BENZENE	No	C19H32	260.47	646.16	341.20	1105.83	614.35
3149	P-METHYLSTYRENE	No	C9H10	118.18	343.00	172.78	802.67	445.93
3149	P-VINYLTOLUENE	No	C9H10	118.18	343.00	172.78	802.67	445.93
3150	2,4-DIMETHYLPENTANE	No	C7H16	100.20	176.90	80.50	636.57	353.65
3151	2,4-DIMETHYL-3-ETHYLPENTANE	No	C9H20	128.25	278.04	136.69	737.71	409.84
3152	2,3-DIMETHYLHEPTANE	No	C9H20	128.25	284.90	140.50	744.57	413.65
3153	2,4-DIMETHYLHEPTANE	No	C9H20	128.25	271.20	132.89	730.87	406.04
3154	2,5-DIMETHYLHEPTANE	No	C9H20	128.25	276.80	136.00	736.47	409.15
3155	2,6-DIMETHYLHEPTANE	No	C9H20	128.25	275.38	135.21	735.05	408.36
3156	2-METHYL-3-ETHYLHEXANE	No	C9H20	128.25	280.40	138.00	740.07	411.15
3157	3-METHYLOCTANE	No	C9H20	128.25	291.58	144.21	751.25	417.36
3158	2,2,4-TRIMETHYLHEXANE	Yes	C9H20	128.25	259.77	126.54	719.44	399.69
3159	2,2,5-TRIMETHYLHEXANE	No	C9H20	128.25	255.35	124.08	715.02	397.23
3160	2,3,3-TRIMETHYLHEXANE	No	C9H20	128.25	279.82	137.68	739.49	410.83
3161	2,3,5-TRIMETHYLHEXANE	No	C9H20	128.25	268.41	131.34	728.08	404.49
3162	2,4,4-TRIMETHYLHEXANE	No	C9H20	128.25	267.17	130.65	726.84	403.80
3163	2,6-DIMETHYLOCTANE	No	C10H22	142.29	317.37	158.54	777.04	431.69
3164	3-METHYLNONANE	No	C10H22	142.29	334.04	167.80	793.71	440.95
3165	2,2,3,3-TETRAMETHYLHEXANE	No	C10H22	142.29	320.56	160.31	780.23	433.46
3166	2,2,4,5-TETRAMETHYLHEXANE	No	C10H22	142.29	298.18	147.88	757.85	421.03
3167	2,2,4-TRIMETHYLHEPTANE	No	C10H22	142.29	298.94	148.30	758.61	421.45
3168	2,2,5-TRIMETHYLHEPTANE	No	C10H22	142.29	303.44	150.80	763.11	423.95
3169	2,2,6-TRIMETHYLHEPTANE	No	C10H22	142.29	300.07	148.93	759.74	422.08
3170	2,4,4-TRIMETHYLHEPTANE	No	C10H22	142.29	303.80	151.00	763.47	424.15
3171	2,5,5-TRIMETHYLHEPTANE	No	C10H22	142.29	307.04	152.80	766.71	425.95
3172	3,3,4-TRIMETHYLHEPTANE	No	C10H22	142.29	323.42	161.90	783.09	435.05
3173	3,4,5-TRIMETHYLHEPTANE	No	C10H22	142.29	324.50	162.50	784.17	435.65
3174	T-BUTYL ETHER	No	C8H18O	130.23	228.20	109.00	687.87	382.15
3174	DI-T-BUTYL ETHER	No	C8H18O	130.23	228.20	109.00	687.87	382.15
3175	1-METHYLNAPHTHALENE	No	C11H10	142.20	472.43	244.68	932.10	517.83
3176	2-METHYLNAPHTHALENE	No	C11H10	142.20	465.90	241.06	925.57	514.21
3177	1-TRIDECANOL	No	C13H28O	200.37	525.23	274.02	984.90	547.17
3177	TRIDECYL ALCOHOL	No	C13H28O	200.37	525.23	274.02	984.90	547.17
3178	1-ETHENYL-2-METHYLBENZENE	No	C9H10	118.17	339.83	171.02	799.50	444.17
3178	O-METHYLSTYRENE	No	C9H10	118.17	339.83	171.02	799.50	444.17
3178	O-VINYLTOLUENE	No	C9H10	118.17	339.83	171.02	799.50	444.17
3179	1-ETHENYL-3-METHYLBENZENE	No	C9H10	118.17	340.88	171.60	800.55	444.75
3179	M-METHYLSTYRENE	No	C9H10	118.17	340.88	171.60	800.55	444.75
3179	M-VINYLTOLUENE	No	C9H10	118.17	340.88	171.60	800.55	444.75
3180	TRANS- $\beta$ -METHYLSTYRENE	No	C9H10	118.17	352.83	178.24	812.50	451.39
3180	TRANS-PROPENYLBENZENE	No	C9H10	118.17	352.83	178.24	812.50	451.39
3181	1-ETHYLNAPHTHALENE	No	C12H12	156.21	497.33	258.52	957.00	531.67
3182	2-ETHYLNAPHTHALENE	No	C12H12	156.21	494.43	256.91	954.10	530.06
3183	1-PROPYLNAPHTHALENE	No	C13H14	170.24	522.53	272.52	982.20	545.67
3184	2-PROPYLNAPHTHALENE	No	C13H14	170.24	524.30	273.50	983.97	546.65
3185	BIACETYLENE	No	C4H2	50.06	50.53	10.29	510.20	283.44
3185	1,3-BUTADIENE	No	C4H2	50.06	50.53	10.29	510.20	283.44
3185	DIACETYLENE	No	C4H2	50.06	50.53	10.29	510.20	283.44
3186	SPIROPENTANE	No	C5H8	68.11	102.13	38.96	561.80	312.11
3187	1-CYCLOPENTYLPROPANE	No	C8H16	112.22	267.71	130.95	727.38	404.10
3187	N-PROPYLCYCLOPENTANE	No	C8H16	112.22	267.71	130.95	727.38	404.10
3188	1-CYCLOHEXYLPROPANE	No	C9H18	126.24	314.03	156.68	773.70	429.83
3188	N-PROPYLCYCLOHEXANE	No	C9H18	126.24	314.03	156.68	773.70	429.83
3189	N-BUTYLCYCLOPENTANE	No	C9H18	126.23	314.83	157.13	774.50	430.28
3190	N-BUTYLCYCLOHEXANE	No	C10H20	140.26	357.70	180.94	817.37	454.09
3190	1-CYCLOHEXYLBUTANE	No	C10H20	140.26	357.70	180.94	817.37	454.09
3191	1-CYCLOPENTYLHEXANE	No	C11H22	154.28	397.23	202.91	856.90	476.06
3191	N-HEXYLCYCLOPENTANE	No	C11H22	154.28	397.23	202.91	856.90	476.06
3192	1-UNDECENE	No	C11H22	154.28	378.81	192.67	838.48	465.82
3193	1-CYCLOPENTYLHEPTANE	No	C12H24	168.31	435.02	223.90	894.69	497.05
3193	N-HEPTYLCYCLOPENTANE	No	C12H24	168.31	435.02	223.90	894.69	497.05
3194	1-TRIDECENE	No	C13H26	182.33	451.00	232.78	910.67	505.93
3195	2-BUTYLNAPHTHALENE	No	C14H16	184.26	552.23	289.02	1011.90	562.17
3196	1-CYCLOPENTYLDECANE	No	C15H30	210.39	534.88	279.38	994.55	552.53
3196	N-DECYLCYCLOPENTANE	No	C15H30	210.39	534.88	279.38	994.55	552.53
3197	1-PENTADECENE	No	C15H30	210.39	515.11	268.39	974.78	541.54
3198	CETYLENE	No	C16H32	224.41	544.73	284.85	1004.40	558.00
3198	1-HEXADECENE	No	C16H32	224.41	544.73	284.85	1004.40	558.00
3199	1-OCTADECENE	No	C18H36	252.49	598.33	314.63	1058.00	587.78

3200	N-HENEICOSANE	No	C21H44	296.58	673.7	356.50	1133.37	629.65
3201	N-DOCOSANE	No	C22H46	310.607	695.48	368.60	1155.15	641.75
3202	N-TRICOSANE	No	C23H48	324.634	716.36	380.20	1176.03	653.35
3203	N-TETRACOSANE	No	C24H50	338.661	736.34	391.30	1196.01	664.45
3204	N-PENTACOSANE	No	C25H52	352.688	755.42	401.90	1215.09	675.05
3205	N-HEXACOSANE	No	C26H54	366.715	773.96	412.20	1233.63	685.35
3206	N-HEPTACOSANE	No	C27H56	380.742	791.78	422.10	1251.45	695.25
3207	N-OCTACOSANE	No	C28H58	394.769	808.88	431.60	1268.55	704.75
3208	N-NONACOSANE	No	C29H60	408.795	825.44	440.80	1285.11	713.95
3209	N-TRIACONTANE	No	C30H62	422.822	841.46	449.70	1301.13	722.85
3211	N-DOTRIACONTANE	No	C32H66	450.876	870.26	465.70	1329.93	738.85
3215	N-HEXATRIACONTANE	No	C36H74	506.984	926.6	497.00	1386.27	770.15

## Component Database - ID From 4000 to 4999

The components ID numbers between 4000-4999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, and vapor pressure (as a function of temperature in range at least from 200 to 760 mmHg). For other properties see *Component Properties Estimation Methods*.

DESIGN		Mixed		Molecular				
II ID	Name	Amine	Formula	Weight	BP (F)	BP (C)	BP (R)	BP (K)
4001	DIMETHOXYMETHANE	No	C3H8O2	76.10	113.99	45.55	573.66	318.70
4001	DIMETHYLFORMAL	No	C3H8O2	76.10	113.99	45.55	573.66	318.70
4001	METHYLAL	No	C3H8O2	76.10	113.99	45.55	573.66	318.70
4002	PENTANOIC ACID	No	C5H10O2	102.13	364.01	184.45	823.68	457.60
4002	N-VALERIC ACID	No	C5H10O2	102.13	364.01	184.45	823.68	457.60
4003	ISOVALERIC ACID	No	C5H10O2	102.13	350.06	176.70	809.73	449.85
4003	3-METHYLBUTANOIC ACID	No	C5H10O2	102.13	350.06	176.70	809.73	449.85
4004	ISOBUTYL PROPANOATE	No	C7H14O2	130.19	278.24	136.80	737.91	409.95
4004	ISOBUTYL PROPIONATE	No	C7H14O2	130.19	278.24	136.80	737.91	409.95
4005	N-PROPYL BUTANOATE	No	C7H14O2	130.19	286.70	141.50	746.37	414.65
4005	N-PROPYL BUTYRATE	No	C7H14O2	130.19	286.70	141.50	746.37	414.65
4006	N-PROPYL ISOBUTYRATE	No	C7H14O2	130.19	275.72	135.40	735.39	408.55
4006	N-PROPYL-2-METHYL PROPANOATE	No	C7H14O2	130.19	275.72	135.40	735.39	408.55
4007	ISOBUTYL BUTANOATE	No	C8H16O2	144.22	313.88	156.60	773.55	429.75
4007	ISOBUTYL BUTYRATE	No	C8H16O2	144.22	313.88	156.60	773.55	429.75
4008	ISOBUTYL ISOBUTYRATE	No	C8H16O2	144.22	299.57	148.65	759.24	421.80
4008	ISOBUTYL-2-METHYL PROPANOATE	No	C8H16O2	144.22	299.57	148.65	759.24	421.80
4009	ISOAMYL BUTYRATE	No	C9H18O2	158.24	353.48	178.60	813.15	451.75
4009	ISOPENTYL BUTANOATE	No	C9H18O2	158.24	353.48	178.60	813.15	451.75
4009	ISOPENTYL BUTYRATE	No	C9H18O2	158.24	353.48	178.60	813.15	451.75
4010	ETHYL ISOVALERATE	No	C7H14O2	130.18	272.84	133.80	732.51	406.95
4010	ETHYL-3-METHYL BUTANOATE	No	C7H14O2	130.18	272.84	133.80	732.51	406.95
4011	N-PROPYL ISOVALERATE	No	C8H16O2	144.22	310.28	154.60	769.95	427.75
4011	N-PROPYL-3-METHYL BUTANOATE	No	C8H16O2	144.22	310.28	154.60	769.95	427.75
4012	ISOBUTYL ISOVALERATE	No	C9H18O2	158.24	334.58	168.10	794.25	441.25
4012	ISOBUTYL-3-METHYL BUTANOATE	No	C9H18O2	158.24	334.58	168.10	794.25	441.25
4013	O-ETHYLPHENOL	No	C8H10O	122.17	400.14	204.52	859.81	477.67
4014	M-ETHYLPHENOL	No	C8H10O	122.17	425.16	218.42	884.83	491.57
4015	P-ETHYLPHENOL	No	C8H10O	122.17	424.38	217.99	884.05	491.14
4016	2,3-DIMETHYL PHENOL	No	C8H10O	122.17	422.37	216.87	882.04	490.02
4016	2,3-XYLENOL	No	C8H10O	122.17	422.37	216.87	882.04	490.02
4017	2,4-DIMETHYL PHENOL	No	C8H10O	122.17	411.68	210.93	871.35	484.08
4017	2,4-XYLENOL	No	C8H10O	122.17	411.68	210.93	871.35	484.08
4018	2,5-DIMETHYL PHENOL	No	C8H10O	122.17	412.04	211.13	871.71	484.28
4018	2,5-XYLENOL	No	C8H10O	122.17	412.04	211.13	871.71	484.28
4019	2,6-DIMETHYL PHENOL	No	C8H10O	122.17	393.85	201.03	853.52	474.18
4019	2,6-XYLENOL	No	C8H10O	122.17	393.85	201.03	853.52	474.18
4020	3,4-DIMETHYL PHENOL	No	C8H10O	122.17	440.50	226.94	900.17	500.09
4020	3,4-XYLENOL	No	C8H10O	122.17	440.50	226.94	900.17	500.09
4021	3,5-XYLENOL	No	C8H10O	122.17	431.05	221.69	890.72	494.84
4022	PARALDEHYDE	No	C6H12O3	132.16	255.29	124.05	714.96	397.20
4022	2,4,6-TRIMETHYL-1,3,5-TRIOXANE	No	C6H12O3	132.16	255.29	124.05	714.96	397.20
4023	DIISOAMYL SULFIDE	No	C10H22S	174.35	420.80	216.00	880.47	489.15
4023	2,8-DIMETHYL-5-THIANONANE	No	C10H22S	174.35	420.80	216.00	880.47	489.15
4023	ISOPENTYL SULFIDE	No	C10H22S	174.35	420.80	216.00	880.47	489.15
4024	DIALLYL SULFIDE	No	C6H10S	114.21	281.66	138.70	741.33	411.85
4024	4-THIA-1,5-HEPTADIENE	No	C6H10S	114.21	281.66	138.70	741.33	411.85
4025	AZOLE	No	C4H5N	67.09	265.64	129.80	725.31	402.95
4025	PYRROLE	No	C4H5N	67.09	265.64	129.80	725.31	402.95

## Chapter 2

4026	4-METHYL PYRIDINE	No	C6H7N	93.13	293.64	145.36	753.31	418.51
4026	4-PICOLINE	No	C6H7N	93.13	293.64	145.36	753.31	418.51
4027	2,4-DIMETHYL PYRIDINE	No	C7H9N	107.16	317.13	158.41	776.80	431.56
4027	2,4-LUTIDINE	No	C7H9N	107.16	317.13	158.41	776.80	431.56
4028	QUINOLINE	No	C9H7N	129.16	459.95	237.75	919.62	510.90
4029	ISOQUINOLINE	No	C9H7N	129.16	464.99	240.55	924.66	513.70
4030	DIETHYLENE GLYCOL	No	C4H10O3	106.12	474.44	245.80	934.11	518.95
4030	DEG	No	C4H10O3	106.12	474.44	245.80	934.11	518.95
4030	2-HYDROXYETHYL ETHER	No	C4H10O3	106.12	474.44	245.80	934.11	518.95
4031	1,2-PROPANEDIOL	No	C3H8O2	76.10	369.14	187.30	828.81	460.45
4031	PROPYLENE GLYCOL	No	C3H8O2	76.10	369.14	187.30	828.81	460.45
4031	PEG	No	C3H8O2	76.10	369.14	187.30	828.81	460.45
4032	1,3-PROPANEDIOL	No	C3H8O2	76.11	417.92	214.40	877.59	487.55
4033	1,3-BUTANEDIOL	No	C4H10O2	90.12	404.60	207.00	864.27	480.15
4034	1,4-BUTANEDIOL	No	C4H10O2	90.12	442.40	228.00	902.07	501.15
4035	2,3-BUTANEDIOL	No	C4H10O2	90.12	357.26	180.70	816.93	453.85
4036	1,5-PENTANEDIOL	No	C5H12O2	104.15	462.20	239.00	921.87	512.15
4037	DIETHYLENE GLYCOL DIMETHYL ETHER	No	C6H14O3	134.17	319.37	159.65	779.04	432.80
4037	DIGLYME	No	C6H14O3	134.17	319.37	159.65	779.04	432.80
4037	DI(2-METHOXYETHYL)ETHER	No	C6H14O3	134.17	319.37	159.65	779.04	432.80
4037	BIS(2-METHOXYETHYL)ETHER	No	C6H14O3	134.17	319.37	159.65	779.04	432.80
4038	N-METHYL-2-PYRROLIDONE	No	C5H9NO	99.10	395.60	202.00	855.27	475.15
4038	M-PYROL	No	C5H9NO	99.10	395.60	202.00	855.27	475.15
4038	NMP	No	C5H9NO	99.10	395.60	202.00	855.27	475.15
4039	ACETAL	No	C6H14O2	118.18	216.05	102.25	675.72	375.40
4039	ACETALDEHYDE DIETHYL ACETAL	No	C6H14O2	118.18	216.05	102.25	675.72	375.40
4039	1,1-DIETHOXYETHANE	No	C6H14O2	118.18	216.05	102.25	675.72	375.40
4039	ETHYLIDENE DIETHYL ETHER	No	C6H14O2	118.18	216.05	102.25	675.72	375.40
4040	2,3-DIMETHYL PYRIDINE	No	C7H9N	107.16	321.26	160.70	780.93	433.85
4040	2,3-LUTIDINE	No	C7H9N	107.16	321.26	160.70	780.93	433.85
4041	2,5-DIMETHYL PYRIDINE	No	C7H9N	107.16	314.61	157.01	774.28	430.16
4041	2,5-LUTIDINE	No	C7H9N	107.16	314.61	157.01	774.28	430.16
4042	3,4-DIMETHYL PYRIDINE	No	C7H9N	107.16	354.44	179.13	814.11	452.28
4042	3,4-LUTIDINE	No	C7H9N	107.16	354.44	179.13	814.11	452.28
4043	3,5-DIMETHYL PYRIDINE	No	C7H9N	107.16	340.88	171.60	800.55	444.75
4043	3,5-LUTIDINE	No	C7H9N	107.16	340.88	171.60	800.55	444.75
4044	TRIETHYLENE GLYCOL	No	C6H14O4	150.17	532.94	278.30	992.61	551.45
4044	TEG	No	C6H14O4	150.17	532.94	278.30	992.61	551.45
4045	ACETOPHENONE	No	C8H8O	120.14	395.24	201.80	854.91	474.95
4045	METHYL PHENYL KETONE	No	C8H8O	120.14	395.24	201.80	854.91	474.95
4046	MESITYL OXIDE	No	C6H10O	98.15	265.57	129.76	725.24	402.91
4046	4-METHYL-3-PENTENE-2-ONE	No	C6H10O	98.15	265.57	129.76	725.24	402.91
4047	ADIPIC ACID	No	C6H10O4	146.14	639.50	337.50	1099.17	610.65
4047	HEXANEDIOIC ACID	No	C6H10O4	146.14	639.50	337.50	1099.17	610.65
4048	N-BUTYL ACRYLATE	No	C7H12O2	128.17	297.32	147.40	756.99	420.55
4048	BUTYL PROPENOATE	No	C7H12O2	128.17	297.32	147.40	756.99	420.55
4049	P-CHLORONITROBENZENE	No	C6H4CLNO2	157.56	467.60	242.00	927.27	515.15
4049	1-CHLORO-4-NITROBENZENE	No	C6H4CLNO2	157.56	467.60	242.00	927.27	515.15
4050	BENZYL CHLORIDE	No	C7H7CL	126.59	354.74	179.30	814.41	452.45
4050	$\alpha$ -CHLOROTOLUENE	No	C7H7CL	126.59	354.74	179.30	814.41	452.45
4051	DIETHANOLAMINE	Yes	C4H11NO2	105.14	514.40	268.00	974.07	541.15
4051	DIETHYL-2,2'-DIHYDROXYAMINE	Yes	C4H11NO2	105.14	514.40	268.00	974.07	541.15
4051	DEA	Yes	C4H11NO2	105.14	514.40	268.00	974.07	541.15
4052	$\alpha$ -DICYCLOPENTADIENE (ENDO)	No	C10H12	132.21	338.00	170.00	797.67	443.15
4053	ETHYL ACRYLATE	No	C5H8O2	100.13	211.64	99.80	671.31	372.95
4054	2-ETHYL-1-HEXANOL	No	C8H18O	130.23	365.00	185.00	824.67	458.15
4055	1,2-DIAMINOETHANE	No	C2H8N2	60.11	241.70	116.50	701.37	389.65
4055	ETHYLENE DIAMINE	No	C2H8N2	60.11	241.70	116.50	701.37	389.65
4056	1,1-DIBROMOETHANE	No	C2H4BR2	187.87	229.40	109.67	689.07	382.82
4056	ETHYLIDENE DIBROMIDE	No	C2H4BR2	187.87	229.40	109.67	689.07	382.82
4057	ETHYLENE GLYCOL MONOMETHYL ETHER	No	C3H8O2	76.09	255.97	124.43	715.64	397.58
4057	2-METHOXYETHANOL	No	C3H8O2	76.09	255.97	124.43	715.64	397.58
4058	CIS-BUTENEDIOIC ACID	No	C4H4O4	116.07	275.00	135.00	734.67	408.15
4058	MALEIC ACID	No	C4H4O4	116.07	275.00	135.00	734.67	408.15
4059	TRANS-BUTENEDIOIC ACID	No	C4H4O4	116.07	554.00	290.00	1013.67	563.15
4059	FUMARIC ACID	No	C4H4O4	116.07	554.00	290.00	1013.67	563.15
4060	ISOOCTYL ALCOHOL	No	C8H18O	130.22	367.70	186.50	827.37	459.65
4060	6-METHYL-1-HEPTANOL	No	C8H18O	130.22	367.70	186.50	827.37	459.65
4061	2-OCTANOL	No	C8H18O	130.22	356.00	180.00	815.67	453.15
4062	NITROBENZENE	No	C6H5NO2	123.11	411.53	210.85	871.20	484.00
4063	4-METHYL-1,3-DIOXOLAN-2-ONE	No	C4H6O3	102.09	467.60	242.00	927.27	515.15

4063	1,2-PROPANEDIOL CARBONATE	No	C4H6O3	102.09	467.60	242.00	927.27	515.15
4063	PROPYLENE CARBONATE	No	C4H6O3	102.09	467.60	242.00	927.27	515.15
4064	CARBON TETRABROMIDE	No	CBR4	331.65	373.10	189.50	832.77	462.65
4064	TETRABROMOMETHANE	No	CBR4	331.65	373.10	189.50	832.77	462.65
4065	BROMOFORM	No	CHBR3	252.75	301.10	149.50	760.77	422.65
4065	TRIBROMOMETHANE	No	CHBR3	252.75	301.10	149.50	760.77	422.65
4066	ISOBUTYRONITRILE	No	C4H7N	69.10	218.50	103.61	678.17	376.76
4066	ISOPROPYL CYANIDE	No	C4H7N	69.10	218.50	103.61	678.17	376.76
4067	CUMENE HYDROPEROXIDE	No	C9H12O2	152.19	679.33	359.63	1139.00	632.78
4068	BI-ISOPROPENYL	No	C6H10	82.14	155.80	68.78	615.47	341.93
4068	2,3-DIMETHYL-1,3-BUTADIENE	No	C6H10	82.14	155.80	68.78	615.47	341.93
4069	BI-ALLYL	No	C6H10	82.14	139.03	59.46	598.70	332.61
4069	1,5-HEXADIENE	No	C6H10	82.14	139.03	59.46	598.70	332.61
4070	DIETHYLACETYLENE	No	C6H10	82.14	178.57	81.43	638.24	354.58
4070	3-HEXYNE	No	C6H10	82.14	178.57	81.43	638.24	354.58
4071	SEC-BUTYLBENZENE	No	C10H14	134.22	344.00	173.33	803.67	446.48
4071	2-PHENYLBUTANE	No	C10H14	134.22	344.00	173.33	803.67	446.48
4072	T-BUTYLBENZENE	No	C10H14	134.22	336.47	169.15	796.14	442.30
4072	2-PHENYL-2-METHYLPROPANE	No	C10H14	134.22	336.47	169.15	796.14	442.30
4073	DIISOBUTYLENE	No	C8H16	112.21	214.63	101.46	674.30	374.61
4073	2,4,4-TRIMETHYL-1-PENTENE	No	C8H16	112.21	214.63	101.46	674.30	374.61
4074	$\alpha$ -PINENE	No	C10H16	136.24	313.06	156.14	772.73	429.29
4074	2-PINENE	No	C10H16	136.24	313.06	156.14	772.73	429.29
4074	2,6,6-TRIMETHYL-BICYCLO 3.1.1 HEPT-2-ENE	No	C10H16	136.24	313.06	156.14	772.73	429.29
4075	6,6-DIMETHYL-2-METHYLENE-BICYCLO 3.1.1 HEPTANE	No	C10H16	136.24	330.87	166.04	790.54	439.19
4075	NOPINENE	No	C10H16	136.24	330.87	166.04	790.54	439.19
4075	$\beta$ -PINENE	No	C10H16	136.24	330.87	166.04	790.54	439.19
4076	O-CHLOROPHENOL	No	C6H5CLO	128.56	346.82	174.90	806.49	448.05
4077	P-CHLOROPHENOL	No	C6H5CLO	128.56	428.00	220.00	887.67	493.15
4078	ACETOACETIC ESTER	No	C6H10O3	130.14	357.44	180.80	817.11	453.95
4078	ETHYL ACETOACETATE	No	C6H10O3	130.14	357.44	180.80	817.11	453.95
4078	ETHYL 3-OXO-BUTANOATE	No	C6H10O3	130.14	357.44	180.80	817.11	453.95
4079	CHLOROACETIC ACID	No	C2H3CLO2	94.50	372.38	189.10	832.05	462.25
4079	2-CHLOROETHANOIC ACID	No	C2H3CLO2	94.50	372.38	189.10	832.05	462.25
4080	BENZOYL CHLORIDE	No	C7H5CLO	140.57	386.60	197.00	846.27	470.15
4080	PHENYL CARBONYL CHLORIDE	No	C7H5CLO	140.57	386.60	197.00	846.27	470.15
4081	BENZYL ACETATE	No	C9H10O2	150.17	419.90	215.50	879.57	488.65
4081	BENZYL ETHANOATE	No	C9H10O2	150.17	419.90	215.50	879.57	488.65
4082	BENZYL ALCOHOL	No	C7H8O	108.13	401.64	205.36	861.31	478.51
4082	$\alpha$ -HYDROXY TOLUENE	No	C7H8O	108.13	401.64	205.36	861.31	478.51
4082	PHENYL CARBINOL	No	C7H8O	108.13	401.64	205.36	861.31	478.51
4083	$\alpha$ -AMINOTOLUENE	No	C7H9N	107.16	364.10	184.50	823.77	457.65
4083	BENZYL AMINE	No	C7H9N	107.16	364.10	184.50	823.77	457.65
4084	BIS(2-CHLOROETHYL) ETHER	No	C4H8CL2O	143.02	353.30	178.50	812.97	451.65
4084	2,2'-DI(CHLOROETHYL)ETHER	No	C4H8CL2O	143.02	353.30	178.50	812.97	451.65
4084	DI(CHLOROETHYL)ETHER	No	C4H8CL2O	143.02	353.30	178.50	812.97	451.65
4085	DIPHENYL ETHER	No	C12H10O	170.21	496.40	258.00	956.07	531.15
4085	DIPHENYL OXIDE	No	C12H10O	170.21	496.40	258.00	956.07	531.15
4086	FURFURYL ALCOHOL	No	C5H6O2	98.10	338.00	170.00	797.67	443.15
4086	2-HYDROXYMETHYL FURAN	No	C5H6O2	98.10	338.00	170.00	797.67	443.15
4087	ISOPROPYL ACETATE	No	C5H10O2	102.13	192.20	89.00	651.87	362.15
4087	2-PROPYL ETHANOATE	No	C5H10O2	102.13	192.20	89.00	651.87	362.15
4088	FUSEL OIL	No	C5H12O	88.15	266.90	130.50	726.57	403.65
4088	ISOAMYL ALCOHOL	No	C5H12O	88.15	266.90	130.50	726.57	403.65
4088	ISOPENTYL ALCOHOL	No	C5H12O	88.15	266.90	130.50	726.57	403.65
4088	3-METHYLBUTANOL	No	C5H12O	88.15	266.90	130.50	726.57	403.65
4088	3-METHYL-1-BUTANOL	No	C5H12O	88.15	266.90	130.50	726.57	403.65
4089	3-NITROTOLUENE	No	C7H7NO2	137.13	450.68	232.60	910.35	505.75
4089	M-NITROTOLUENE	No	C7H7NO2	137.13	450.68	232.60	910.35	505.75
4090	2-NITROTOLUENE	No	C7H7NO2	137.13	432.47	222.48	892.14	495.63
4090	O-NITROTOLUENE	No	C7H7NO2	137.13	432.47	222.48	892.14	495.63
4091	4-NITROTOLUENE	No	C7H7NO2	137.13	460.94	238.30	920.61	511.45
4091	P-NITROTOLUENE	No	C7H7NO2	137.13	460.94	238.30	920.61	511.45
4092	4-NITRO-1-AMINO BENZENE	No	C6H6N2O2	138.12	636.80	336.00	1096.47	609.15
4092	4-NITROANILINE	No	C6H6N2O2	138.12	636.80	336.00	1096.47	609.15
4092	P-NITROANILINE	No	C6H6N2O2	138.12	636.80	336.00	1096.47	609.15
4093	1,2,4,5-TETRACHLORO BENZENE	No	C6H2CL4	215.90	473.00	245.00	932.67	518.15
4094	BENZOTRICHLORIDE	No	C7H5CL3	195.48	416.30	213.50	875.97	486.65
4094	PHENYL CHLOROFORM	No	C7H5CL3	195.48	416.30	213.50	875.97	486.65
4094	(1,1,1-TRICHLOROMETHYL) BENZENE	No	C7H5CL3	195.48	416.30	213.50	875.97	486.65

## Chapter 2

4094	$\alpha$ - $\alpha$ - $\alpha$ -TRICHLOROTOLUENE	No	C7H5CL3	195.48	416.30	213.50	875.97	486.65
4095	2-T-BUTYLPHENOL	No	C10H14O	150.22	435.36	224.09	895.03	497.24
4095	O-T-BUTYLPHENOL	No	C10H14O	150.22	435.36	224.09	895.03	497.24
4096	4-T-BUTYLPHENOL	No	C10H14O	150.22	463.69	239.83	923.36	512.98
4096	P-T-BUTYLPHENOL	No	C10H14O	150.22	463.69	239.83	923.36	512.98
4097	2-CHLORO-1-AMINO BENZENE	No	C6H6CLN	127.57	407.84	208.80	867.51	481.95
4097	2-CHLOROANILINE	No	C6H6CLN	127.57	407.84	208.80	867.51	481.95
4097	O-CHLOROANILINE	No	C6H6CLN	127.57	407.84	208.80	867.51	481.95
4098	4-CHLORO-1-AMINO BENZENE	No	C6H6CLN	127.57	446.90	230.50	906.57	503.65
4098	4-CHLOROANILINE	No	C6H6CLN	127.57	446.90	230.50	906.57	503.65
4098	P-CHLOROANILINE	No	C6H6CLN	127.57	446.90	230.50	906.57	503.65
4099	2-CHLORO-1,3-BUTADIENE	No	C4H5CL	88.54	138.46	59.14	598.13	332.29
4099	CHLOROPRENE	No	C4H5CL	88.54	138.46	59.14	598.13	332.29
4100	O-CHLOROSTYRENE	No	C8H7CL	138.60	367.61	186.45	827.28	459.60
4100	O-CHLOROVINYLBENZENE	No	C8H7CL	138.60	367.61	186.45	827.28	459.60
4100	2-CHLORO-1-VINYLBENZENE	No	C8H7CL	138.60	367.61	186.45	827.28	459.60
4101	P-CHLOROSTYRENE	No	C8H7CL	138.60	375.80	191.00	835.47	464.15
4101	P-CHLOROVINYLBENZENE	No	C8H7CL	138.60	375.80	191.00	835.47	464.15
4101	4-CHLORO-1-VINYLBENZENE	No	C8H7CL	138.60	375.80	191.00	835.47	464.15
4102	ETHYL CHLOROACETATE	No	C4H7CLO2	122.55	290.57	143.65	750.24	416.80
4102	ETHYL2-CHLOROETHANOATE	No	C4H7CLO2	122.55	290.57	143.65	750.24	416.80
4103	ISOBUTYRALDEHYDE	No	C4H8O	72.10	147.38	64.10	607.05	337.25
4103	2-METHYLPROPANAL	No	C4H8O	72.10	147.38	64.10	607.05	337.25
4103	2-METHYLPROPIONALDEHYDE	No	C4H8O	72.10	147.38	64.10	607.05	337.25
4104	METHYL ACRYLATE	No	C4H6O2	86.09	176.36	80.20	636.03	353.35
4104	METHYL 2-PROPENOATE	No	C4H6O2	86.09	176.36	80.20	636.03	353.35
4105	2-METHYL-3-BUTYN-2-OL	No	C5H8O	84.11	220.09	104.49	679.76	377.64
4106	METHYLISOBUTYLCARBINOL	No	C6H14O	102.17	269.06	131.70	728.73	404.85
4106	4-METHYL-2-PENTANOL	No	C6H14O	102.17	269.06	131.70	728.73	404.85
4107	2-METHYLBENZYL ALCOHOL	No	C8H10O	122.16	399.20	204.00	858.87	477.15
4107	METHYLPHENYLCARBINOL	No	C8H10O	122.16	399.20	204.00	858.87	477.15
4107	1-PHENYLETHANOL	No	C8H10O	122.16	399.20	204.00	858.87	477.15
4108	1-NAPHTHOL	No	C10H8O	144.18	540.50	282.50	1000.17	555.65
4108	$\alpha$ -NAPHTHOL	No	C10H8O	144.18	540.50	282.50	1000.17	555.65
4109	ALLYL CYANIDE	No	C4H5N	67.09	245.16	118.42	704.83	391.57
4109	$\beta$ -BUTENEONITRILE	No	C4H5N	67.09	245.16	118.42	704.83	391.57
4109	3-BUTENEONITRILE	No	C4H5N	67.09	245.16	118.42	704.83	391.57
4109	VINYL ACETONITRILE	No	C4H5N	67.09	245.16	118.42	704.83	391.57
4110	2-CHLOROETHANOL	No	C2H5CLO	80.52	263.48	128.60	723.15	401.75
4110	ETHYLENE CHLOROHYDRIN	No	C2H5CLO	80.52	263.48	128.60	723.15	401.75
4111	VINYL ACETATE	No	C4H6O2	86.09	162.92	72.73	622.59	345.88
4111	VINYL ETHANOATE	No	C4H6O2	86.09	162.92	72.73	622.59	345.88
4112	DIACETONE	No	C6H12O2	116.16	334.22	167.90	793.89	441.05
4112	DIACETONE ALCOHOL	No	C6H12O2	116.16	334.22	167.90	793.89	441.05
4112	4-HYDROXY-4-METHYL-2-PENTANONE	No	C6H12O2	116.16	334.22	167.90	793.89	441.05
4113	CIS-BUTENOIC ANYHYDRIDE	No	C4H2O3	98.06	395.60	202.00	855.27	475.15
4113	MALEIC ANHYDRIDE	No	C4H2O3	98.06	395.60	202.00	855.27	475.15
4114	ACROLEIN	No	C3H4O	56.06	126.50	52.50	586.17	325.65
4114	ALLYL ALDEHYDE	No	C3H4O	56.06	126.50	52.50	586.17	325.65
4114	ETHYLENE ALDEHYDE	No	C3H4O	56.06	126.50	52.50	586.17	325.65
4114	2-PROPENAL	No	C3H4O	56.06	126.50	52.50	586.17	325.65
4115	5-METHYL-1-HEPTANOL	No	C8H18O	130.22	367.88	186.60	827.55	459.75
4116	4-METHYL-1-HEPTANOL	No	C8H18O	130.22	361.76	183.20	821.43	456.35
4117	3-METHYL-1-HEPTANOL	No	C8H18O	130.22	366.80	186.00	826.47	459.15
4118	2-METHYL-1-HEPTANOL	No	C8H18O	130.22	348.08	175.60	807.75	448.75
4119	METHYL METHACRYLATE	No	C5H8O2	100.11	213.80	101.00	673.47	374.15
4120	2-AMINOETHANOL	No	C2H7NO	61.08	340.53	171.41	800.20	444.56
4120	ETHANOLAMINE	No	C2H7NO	61.08	340.53	171.41	800.20	444.56
4121	ACETYL CHLORIDE	No	C2H3CLO	78.50	123.35	50.75	583.02	323.90
4121	ETHANOYL CHLORIDE	No	C2H3CLO	78.50	123.35	50.75	583.02	323.90
4122	N,N-DIETHYLANILINE	No	C10H15N	149.24	421.28	216.27	880.95	489.42
4122	DIETHYL PHENYL AMINE	No	C10H15N	149.24	421.28	216.27	880.95	489.42
4123	N-ETHYLANILINE	No	C8H11N	121.18	400.53	204.74	860.20	477.89
4123	ETHYL PHENYL AMINE	No	C8H11N	121.18	400.53	204.74	860.20	477.89
4124	T-BUTYL METHYL KETONE	No	C6H12O	100.16	223.33	106.29	683.00	379.44
4124	3,3-DIMETHYL-2-BUTANONE	No	C6H12O	100.16	223.33	106.29	683.00	379.44
4124	PINACOLONE	No	C6H12O	100.16	223.33	106.29	683.00	379.44
4125	1,3-BENZENEDIOL	No	C6H6O2	110.11	529.83	276.57	989.50	549.72
4125	1,3-DIHYDROXYBENZENE	No	C6H6O2	110.11	529.83	276.57	989.50	549.72
4125	RESORCINOL	No	C6H6O2	110.11	529.83	276.57	989.50	549.72
4126	2-NAPHTHOL	No	C10H8O	144.18	549.26	287.37	1008.93	560.52



# Database Components

4126	β-NAPHTHOL	No	C10H8O	144.18	549.26	287.37	1008.93	560.52
4127	1,4-DIISOPROPYLBENZENE	No	C12H18	162.28	410.67	210.37	870.34	483.52
4127	P-DIISOPROPYLBENZENE	No	C12H18	162.28	410.67	210.37	870.34	483.52
4128	1-AMINOCYCLOHEXANE	No	C6H13N	99.18	274.13	134.52	733.80	407.67
4128	CYCLOHEXYL AMINE	No	C6H13N	99.18	274.13	134.52	733.80	407.67
4129	1-PHENYL-1-PROPANONE	No	C9H10O	134.18	423.46	217.48	883.13	490.63
4129	PROPIOPHENONE	No	C9H10O	134.18	423.46	217.48	883.13	490.63
4130	4-ETHYLANILINE	No	C8H11N	121.18	424.03	217.79	883.70	490.94
4130	P-ETHYLANILINE	No	C8H11N	121.18	424.03	217.79	883.70	490.94
4131	2-MERCAPTOTOLUENE	No	C7H8S	124.22	381.56	194.20	841.23	467.35
4131	2-THIOCREOSOL	No	C7H8S	124.22	381.56	194.20	841.23	467.35
4131	O-THIOCREOSOL	No	C7H8S	124.22	381.56	194.20	841.23	467.35
4131	O-TOLUENETHIOL	No	C7H8S	124.22	381.56	194.20	841.23	467.35
4131	O-TOLYLMERCAPTAN	No	C7H8S	124.22	381.56	194.20	841.23	467.35
4132	3-MERCAPTOTOLUENE	No	C7H8S	124.22	383.23	195.13	842.90	468.28
4132	3-THIOCREOSOL	No	C7H8S	124.22	383.23	195.13	842.90	468.28
4132	M-THIOCREOSOL	No	C7H8S	124.22	383.23	195.13	842.90	468.28
4132	M-TOLUENETHIOL	No	C7H8S	124.22	383.23	195.13	842.90	468.28
4132	M-TOLYLMERCAPTAN	No	C7H8S	124.22	383.23	195.13	842.90	468.28
4133	4-MERCAPTOTOLUENE	No	C7H8S	124.22	383.03	195.02	842.70	468.17
4133	4-THIOCREOSOL	No	C7H8S	124.22	383.03	195.02	842.70	468.17
4133	P-THIOCREOSOL	No	C7H8S	124.22	383.03	195.02	842.70	468.17
4133	P-TOLUENETHIOL	No	C7H8S	124.22	383.03	195.02	842.70	468.17
4133	P-TOLYLMERCAPTAN	No	C7H8S	124.22	383.03	195.02	842.70	468.17
4134	2-ETHYLBENZENETHIOL	No	C8H10O	138.23	410.03	210.02	869.70	483.17
4134	2-ETHYLTHIOPHENOL	No	C8H10O	138.23	410.03	210.02	869.70	483.17
4134	O-MERCAPTOETHYLBENZENE	No	C8H10O	138.23	410.03	210.02	869.70	483.17
4135	CHLORAL	No	C2HCL3O	147.39	207.95	97.75	667.62	370.90
4135	TRICHLOROACETALDEHYDE	No	C2HCL3O	147.39	207.95	97.75	667.62	370.90
4135	2,2,2-TRICHLOROETHANAL	No	C2HCL3O	147.39	207.95	97.75	667.62	370.90
4136	N,N-DIMETHYL FORMAMIDE	No	C3H7NO	73.09	305.63	152.02	765.30	425.17
4136	N,N-DIMETHYL METHANAMIDE	No	C3H7NO	73.09	305.63	152.02	765.30	425.17
4137	CAPROIC ACID	No	C6H12O2	116.16	402.23	205.68	861.90	478.83
4137	HEXANOIC ACID	No	C6H12O2	116.16	402.23	205.68	861.90	478.83
4138	ENANTHIC ACID	No	C7H14O2	130.19	433.33	222.96	893.00	496.11
4138	HEPTANOIC ACID	No	C7H14O2	130.19	433.33	222.96	893.00	496.11
4139	CAPRYLIC ACID	No	C8H16O2	144.22	463.83	239.91	923.50	513.06
4139	OCTANOIC ACID	No	C8H16O2	144.22	463.83	239.91	923.50	513.06
4140	NONANOIC ACID	No	C9H18O2	158.24	492.13	255.63	951.80	528.78
4140	PELARGONIC ACID	No	C9H18O2	158.24	492.13	255.63	951.80	528.78
4141	CAPRIC ACID	No	C10H20O2	172.27	518.03	270.02	977.70	543.17
4141	DECANOIC ACID	No	C10H20O2	172.27	518.03	270.02	977.70	543.17
4142	HENDECANOIC ACID	No	C11H22O2	186.30	543.53	284.18	1003.20	557.33
4142	UNDECANOIC ACID	No	C11H22O2	186.30	543.53	284.18	1003.20	557.33
4143	DODECANOIC ACID	No	C12H24O2	200.33	569.63	298.68	1029.30	571.83
4143	LAURIC ACID	No	C12H24O2	200.33	569.63	298.68	1029.30	571.83
4144	TRIDECANOIC ACID	No	C13H26O2	214.35	593.83	312.13	1053.50	585.28
4145	MYRISTIC ACID	No	C14H28O2	228.38	619.13	326.18	1078.80	599.33
4145	TETRADECANOIC ACID	No	C14H28O2	228.38	619.13	326.18	1078.80	599.33
4146	PENTADECANOIC ACID	No	C15H30O2	242.41	642.03	338.91	1101.70	612.06
4147	HEXADECANOIC ACID	No	C16H32O2	256.43	663.83	351.02	1123.50	624.17
4147	PALMITIC ACID	No	C16H32O2	256.43	663.83	351.02	1123.50	624.17
4148	MARGARIC ACID	No	C17H34O2	270.46	685.43	363.02	1145.10	636.17
4149	OCTADECANOIC ACID	No	C18H36O2	284.50	707.03	375.02	1166.70	648.17
4149	STEARIC ACID	No	C18H36O2	284.50	707.03	375.02	1166.70	648.17
4150	ARACHIDIC ACID	No	C20H40O2	312.54	746.63	397.02	1206.30	670.17
4150	EICOSANOIC ACID	No	C20H40O2	312.54	746.63	397.02	1206.30	670.17
4151	1-ISOPROPYLNAPHTHALENE	No	C13H14	170.24	514.03	267.79	973.70	540.94
4152	2-ISOPROPYLNAPHTHALENE	No	C13H14	170.24	514.73	268.18	974.40	541.33
4153	ACENAPHTHENE	No	C12H10	154.23	534.23	279.02	993.90	552.17
4153	NAPHTHYLENE-ETHYLENE	No	C12H10	154.23	534.23	279.02	993.90	552.17
4154	ANTHRAQUINONE	No	C14H8O2	208.23	715.63	379.79	1175.30	652.94
4155	2-AMINOETHANOL	Yes	C2H7NO	61.09	340.53	171.41	800.20	444.56
4155	ETHANOLAMINE	Yes	C2H7NO	61.09	340.53	171.41	800.20	444.56
4155	MEA	Yes	C2H7NO	61.09	340.53	171.41	800.20	444.56
4155	MONOETHANOLAMINE	Yes	C2H7NO	61.09	340.53	171.41	800.20	444.56
4156	ANTHRACENE	No	C14H10	178.24	647.63	342.02	1107.30	615.17
4157	PHENANTHRENE	No	C14H10	178.24	642.93	339.41	1102.60	612.56
4158	1,2-BENZENEDIOL	No	C6H6O2	110.11	474.13	245.63	933.80	518.78
4158	CATECHOL	No	C6H6O2	110.11	474.13	245.63	933.80	518.78

## Chapter 2

4158	1,2-DIHYDROXYBENZENE	No	C6H6O2	110.11	474.13	245.63	933.80	518.78
4158	PYROCATECHOL	No	C6H6O2	110.11	474.13	245.63	933.80	518.78
4159	2,4,6-TRICHLOROPHENOL	No	C6H3CL3O	197.45	474.83	246.02	934.50	519.17
4160	METHYL CAPROATE	No	C7H14O2	130.19	304.23	151.24	763.90	424.39
4160	METHYL HEXANOATE	No	C7H14O2	130.19	304.23	151.24	763.90	424.39
4161	METHYL CAPRYLATE	No	C9H18O2	158.24	379.43	193.02	839.10	466.17
4161	METHYL OCTANOATE	No	C9H18O2	158.24	379.43	193.02	839.10	466.17
4162	2,3-BENZINDENE	No	C13H10	166.23	568.43	298.02	1028.10	571.17
4162	DIPHENYLENEMETHANE	No	C13H10	166.23	568.43	298.02	1028.10	571.17
4162	FLUORENE	No	C13H10	166.23	568.43	298.02	1028.10	571.17
4163	1,3-CYCLOHEXADIENE	No	C6H8	80.14	176.93	80.52	636.60	353.67
4163	1,2-DIHYDROBENZENE	No	C6H8	80.14	176.93	80.52	636.60	353.67
4164	DIVINYLACETYLENE	No	C6H6	78.12	185.03	85.02	644.70	358.17
4164	1,5-HEXADIEN-3-YNE	No	C6H6	78.12	185.03	85.02	644.70	358.17
4165	2-AMINOPROPANE	No	C3H9N	59.11	90.33	32.41	550.00	305.56
4165	ISOPROPYL AMINE	No	C3H9N	59.11	90.33	32.41	550.00	305.56
4166	ETHYL BUTYL ETHER	No	C6H14O	102.18	197.96	92.20	657.63	365.35
4167	2,3,3-TRIMETHYLBUTENE	No	C7H14	98.19	172.23	77.91	631.90	351.06
4167	TRIPTENE	No	C7H14	98.19	172.23	77.91	631.90	351.06
4168	METHYL BENZOATE	No	C8H8O2	136.16	390.56	199.20	850.23	472.35
4169	2-CYCLOPENTYLPROPANE	No	C8H16	112.22	259.56	126.42	719.23	399.57
4169	ISOPROPYLCYCLOPENTANE	No	C8H16	112.22	259.56	126.42	719.23	399.57
4170	TRANS-2-OCTENE	No	C8H16	112.22	257.00	125.00	716.67	398.15
4171	ETHYL BENZOATE	No	C9H10O2	150.18	414.33	212.41	874.00	485.56
4172	2-CYCLOHEXYLPROPANE	No	C9H18	126.24	310.10	154.50	769.77	427.65
4172	ISOPROPYLCYCLOHEXANE	No	C9H18	126.24	310.10	154.50	769.77	427.65
4173	M-CYMENE	No	C10H14	134.22	347.25	175.14	806.92	448.29
4173	1-ISOPROPYL-3-METHYLBENZENE	No	C10H14	134.22	347.25	175.14	806.92	448.29
4174	O-CYMENE	No	C10H14	134.22	352.67	178.15	812.34	451.30
4174	1-ISOPROPYL-2-METHYLBENZENE	No	C10H14	134.22	352.67	178.15	812.34	451.30
4175	1-CYCLOHEXYL-2-METHYLPROPANE	No	C10H20	140.26	340.43	171.35	800.10	444.50
4175	ISOBUTYLCYCLOHEXANE	No	C10H20	140.26	340.43	171.35	800.10	444.50
4176	SEC-BUTYLCYCLOHEXANE	No	C10H20	140.26	354.80	179.33	814.47	452.48
4176	2-CYCLOHEXYLBUTANE	No	C10H20	140.26	354.80	179.33	814.47	452.48
4177	TERT-BUTYLCYCLOHEXANE	No	C10H20	140.26	340.86	171.59	800.53	444.74
4177	2-CYCLOHEXYL-2-METHYLPROPANE	No	C10H20	140.26	340.86	171.59	800.53	444.74
4178	DIPHENYLMETHANE	No	C13H12	168.25	507.69	264.27	967.36	537.42
4178	DITAN	No	C13H12	168.25	507.69	264.27	967.36	537.42
4178	1,1'-METHYLENEBISBENZENE	No	C13H12	168.238	507.69	264.27	967.36	537.42
4178	DIPHENYLMETHANE	No	C13H12	168.238	507.69	264.27	967.36	537.42
4178	BENZYL BENZENE	No	C13H12	168.238	507.69	264.27	967.36	537.42
4179	1-TERT-BUTYLNAPHTHALENE	No	C14H16	184.26	532.93	278.29	992.60	551.44
4180	2-TERT-BUTYLNAPHTHALENE	No	C14H16	184.26	536.23	280.13	995.90	553.28
4181	METHYL DODECANOATE	No	C13H26O2	214.35	503.63	262.02	963.30	535.17
4181	METHYL LAURATE	No	C13H26O2	214.35	503.63	262.02	963.30	535.17
4182	GLYCEROL	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4182	1,2,3-PROPANETRIOL	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4182	GLYCERIN	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4182	GLYCYL ALCOHOL	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4182	1,2,3-TRIHYDROXYPROPANE	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4182	GLYCERITOL	No	C3H8O3	92.10	550.13	287.85	1009.80	561.00
4183	OLEIC ACID	No	C18H34O2	282.47	679.73	359.85	1139.40	633.00
4183	9-OCTADECENOIC ACID	No	C18H34O2	282.47	679.73	359.85	1139.40	633.00

## Component Database - ID From 5000 to 5999

The components ID numbers between 5000-5999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, heat capacity, critical temperature, and critical pressure. For other properties see *Component Properties Estimation Methods*.

DESIGN		Mixed		Molecular				
II ID	Name	Amine	Formula	Weight	BP (F)	BP (C)	BP (R)	BP (K)
5001	BUTYL ETHER	No	C8H18O	130.22	288.41	142.45	748.08	415.6
5002	HEXAFLUOROBENZENE	No	C6F6	186.06	176.47	80.26	636.14	353.41
5003	NAPHTHALENE	No	C10H8	128.18	424.30	217.94	883.97	491.09

## Component Database - ID From 6000 to 6999

The components ID numbers between 6000-6999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, critical temperature, and critical pressure. For other properties see *Component Properties Estimation Methods*.

DESIGN		Mixed		Molecular				
II ID	Name	Amine	Formula	Weight	BP (F)	BP (C)	BP (R)	BP (K)
6001	PERFLUORO-N-HEXANE	No	C6F14	338.04	134.87	57.15	594.54	330.30
6002	1,2-DIMETHOXYETHANE	No	C4H10O2	90.12	184.10	84.50	643.77	357.65
6002	1,2-ETHANEDIOL DIMETHYL ETHER	No	C4H10O2	90.12	184.10	84.50	643.77	357.65
6002	ETHYLENE GLYCOL DIMETHYL ETHER	No	C4H10O2	90.12	184.10	84.50	643.77	357.65
6003	CL2FC-CFCL2	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6003	1,1,1,2-TETRACHLORO-1,2-DIFLUOROETHANE	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6003	1,2-DIFLUORO-1,2,2,2-TETRACHLOROETHANE	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6003	REFRIGERANT 112A	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6003	R112A	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6003	R-112A	No	C2CL4F2	203.83	197.69	92.05	657.36	365.20
6004	PERFLUORO-N-PROPANE	No	C3F8	188.02	-36.40	-38.00	423.27	235.15
6005	TRIFLUOROACETIC ACID	No	C2HF3O2	114.02	162.32	72.40	621.99	345.55
6005	TRIFLUOROETHANOIC ACID	No	C2HF3O2	114.02	162.32	72.40	621.99	345.55
6006	DI-N-PROPYLAMINE	No	C6H15N	101.19	228.56	109.20	688.23	382.35
6007	METHYL PENTANOATE	No	C6H12O2	116.16	261.14	127.30	720.81	400.45
6007	METHYL VALERATE	No	C6H12O2	116.16	261.14	127.30	720.81	400.45
6008	AMYL FORMATE	No	C6H12O2	116.16	266.72	130.40	726.39	403.55
6008	N-PENTYL FORMATE	No	C6H12O2	116.16	266.72	130.40	726.39	403.55
6008	N-PENTYL METHANOATE	No	C6H12O2	116.16	266.72	130.40	726.39	403.55
6009	PENTAFLUOROBENZENE	No	C6F5H	168.07	185.10	85.06	644.77	358.21
6010	HEXAFLUOROACETONE	No	C3F6O	166.02	-18.49	-28.05	441.18	245.10
6010	PERFLUOROACETONE	No	C3F6O	166.02	-18.49	-28.05	441.18	245.10
6011	PENTAFLUOROCHLOROACETONE	No	C3CLF5O	182.48	46.04	7.80	505.71	280.95
6012	DIISOPROPANOLAMINE	Yes	C6H15NO2	133.19	478.13	247.85	937.80	521.00
6012	DIPA	Yes	C6H15NO2	133.19	478.13	247.85	937.80	521.00

## Component Database - ID From 7000 to 7999

The components ID numbers between 7000-7999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, and heat capacity. For other properties see *Component Properties Estimation Methods*.

DESIGN		Mixed		Molecular				
II ID	Name	Amine	Formula	Weight	BP (F)	BP (C)	BP (R)	BP (K)
7001	1,2-DIIODOPROPANE	No	C3H6I2	295.89	401.00	205.00	860.67	478.15
7002	T-BUTYL IODIDE	No	C4H9I	184.02	-36.67	-38.15	423.00	235.00
7002	2-IODO-2-METHYL PROPANE	No	C4H9I	184.02	-36.67	-38.15	423.00	235.00
7003	SEC-BUTYL ETHER	No	C8H18O	130.22	249.80	121.00	709.47	394.15
7004	2-AMINOBTANE	No	C4H11N	73.14	145.13	62.85	604.80	336.00
7004	SEC-BUTYLAMINE	No	C4H11N	73.14	145.13	62.85	604.80	336.00
7005	T-BUTYL AMINE	No	C4H11N	73.14	112.01	44.45	571.68	317.60
7006	2-FLUOROPROPANE	No	C3H7F	62.09	15.17	-9.35	474.84	263.80
7007	P-DIFLUOROBENZENE	No	C6H4F2	114.09	191.93	88.85	651.60	362.00
7008	1,3-DICHLOROPROPANE	No	C3H6CL2	112.99	248.81	120.45	708.48	393.60
7009	2,2-DICHLOROPROPANE	No	C3H6CL2	112.99	158.99	70.55	618.66	343.70
7010	1-CHLORO-3-METHYL BUTANE	No	C5H11CL	106.59	208.85	98.25	668.52	371.40
7010	ISOAMYL CHLORIDE	No	C5H11CL	106.59	208.85	98.25	668.52	371.40
7011	T-AMYL CHLORIDE	No	C5H11CL	106.59	186.13	85.63	645.80	358.78
7011	2-CHLORO-2-METHYL BUTANE	No	C5H11CL	106.59	186.13	85.63	645.80	358.78
7012	2-BROMOBUTANE	No	C4H9BR	137.02	196.23	91.24	655.90	364.39
7013	2,3-DIBROMO-2-METHYL BUTANE	No	C5H10BR2	229.96	339.53	170.85	799.20	444.00
7014	ALLYL BROMIDE	No	C3H5BR	120.98	159.44	70.80	619.11	343.95
7014	3-BROMO-1-PROPENE	No	C3H5BR	120.98	159.44	70.80	619.11	343.95
7015	1,2-DIIODOETHANE	No	C2H4I2	281.87	391.73	199.85	851.40	473.00
7016	METHYL PENTYL SULFIDE	No	C6H14S	118.23	292.73	144.85	752.40	418.00
7017	HEXYL METHYL SULFIDE	No	C7H16S	132.26	339.53	170.85	799.20	444.00
7018	HEPTYL METHYL SULFIDE	No	C8H18S	146.29	382.73	194.85	842.40	468.00
7019	METHYL OCTYL SULFIDE	No	C9H20S	160.31	424.13	217.85	883.80	491.00
7019	2-THIADECANE	No	C9H20S	160.31	424.13	217.85	883.80	491.00
7020	METHYL NONYL SULFIDE	No	C10H22S	174.34	463.73	239.85	923.40	513.00
7020	2-THIAUNDECANE	No	C10H22S	174.34	463.73	239.85	923.40	513.00
7021	PENTYL SULFIDE	No	C10H22S	174.34	446.18	230.10	905.85	503.25

## Chapter 2

7022	DECYL METHYL SULFIDE	No	C11H24S	188.36	499.91	259.95	959.58	533.10
7022	2-THIADODECANE	No	C11H24S	188.36	499.91	259.95	959.58	533.10
7023	METHYL UNDECYL SULFIDE	No	C12H26S	202.39	533.93	278.85	993.60	552.00
7023	2-THIATRIDEDECANE	No	C12H26S	202.39	533.93	278.85	993.60	552.00
7024	DODECYL METHYL SULFIDE	No	C13H28S	216.42	566.33	296.85	1026.00	570.00
7024	2-THIATETRADECANE	No	C13H28S	216.42	566.33	296.85	1026.00	570.00
7025	METHYL TRIDECYL SULFIDE	No	C14H30S	230.44	596.93	313.85	1056.60	587.00
7025	2-THIAPENTADECANE	No	C14H30S	230.44	596.93	313.85	1056.60	587.00
7026	METHYL TETRADECYL SULFIDE	No	C15H32S	244.47	623.73	328.74	1083.40	601.89
7027	METHYL PENTADECYL SULFIDE	No	C16H34S	258.49	652.73	344.85	1112.40	618.00
7028	HEXADECYL METHYL SULFIDE	No	C17H36S	272.52	677.93	358.85	1137.60	632.00
7029	HEPTADECYL METHYL SULFIDE	No	C18H38S	286.55	703.13	372.85	1162.80	646.00
7030	METHYL OCTADECYL SULFIDE	No	C19H40S	300.57	726.53	385.85	1186.20	659.00
7031	METHYL NONADECYL SULFIDE	No	C20H42S	314.60	748.13	397.85	1207.80	671.00
7032	CARBONYL FLUORIDE	No	CF2O	66.01	-117.85	-83.25	341.82	189.90
7033	METHYL T-BUTYL ETHER	No	C5H12O	88.15	131.36	55.20	591.03	328.35
7034	AZIRIDINE	No	C2H5N	43.07	132.53	55.85	592.20	329.00
7034	DIHYDROAZIRINE	No	C2H5N	43.07	132.53	55.85	592.20	329.00
7034	ETHYLENE IMINE	No	C2H5N	43.07	132.53	55.85	592.20	329.00
7035	METHYL NITRITE	No	CH3NO2	61.04	0.77	-17.35	460.44	255.80
7036	METHYL NITRATE	No	CH3NO3	77.04	148.37	64.65	608.04	337.80
7037	ETHYL NITRATE	No	C2H5NO3	91.07	189.77	87.65	649.44	360.80
7038	PROPYL NITRATE	No	C3H7NO3	105.09	230.09	110.05	689.76	383.20
7039	IODOFORM	No	CHI3	393.74	424.33	217.96	884.00	491.11
7039	TRIIODOMETHANE	No	CHI3	393.74	424.33	217.96	884.00	491.11
7040	ALLYL IODIDE	No	C3H5I	167.98	215.33	101.85	675.00	375.00
7040	3-IODO-1-PROPENE	No	C3H5I	167.98	215.33	101.85	675.00	375.00
7041	HEPTYL SULFIDE	No	C14H30S	230.44	286.43	141.35	746.10	414.50
7042	ETHANETHIOLIC ACID	No	C2H4SO	76.12	188.60	87.00	648.27	360.15
7042	THIOACETIC ACID	No	C2H4SO	76.12	188.60	87.00	648.27	360.15
7042	THIOLOACETIC ACID	No	C2H4SO	76.12	188.60	87.00	648.27	360.15
7043	CYCLOHEXENE	No	C6H10	82.14	181.36	82.98	641.03	356.13
7044	N-BUTYLACETYLENE	No	C6H10	82.14	160.39	71.33	620.06	344.48
7044	1-HEXYNE	No	C6H10	82.14	160.39	71.33	620.06	344.48
7045	1-METHYLCYCLOPENTENE	No	C6H10	82.14	167.88	75.49	627.55	348.64
7046	3-METHYLCYCLOPENTENE	No	C6H10	82.14	148.84	64.91	608.51	338.06
7047	4-METHYLCYCLOPENTENE	No	C6H10	82.14	150.21	65.67	609.88	338.82
7048	1-BUTEN-2-YNE	Yes	C4H4	52.07	41.63	5.35	501.30	278.50
7048	VINYLCACETYLENE	Yes	C4H4	52.07	41.63	5.35	501.30	278.50
7049	1,3,5-TRIETHYLBENZENE	No	C12H18	162.28	419.03	215.02	878.70	488.17
7050	CIS- $\beta$ -METHYL STYRENE	No	C9H10	118.17	333.31	167.39	792.98	440.54
7050	CIS-PROPENYLBENZENE	No	C9H10	118.17	333.31	167.39	792.98	440.54
7051	METHYLDIETHANOLAMINE	Yes	C5H13NO2	119.16	477.23	247.35	936.90	520.50
7051	MDEA	Yes	C5H13NO2	119.16	477.23	247.35	936.90	520.50

## Component Database - ID From 8000 to 8999

The components ID numbers between 8000-8999 in DESIGN II database have the name, structure, molecular weight, normal boiling point, and liquid density. For other properties see *Component Properties Estimation Methods*.

DESIGN II ID	Name	Mixed Amine	Formula	Molecular Weight	BP (F)	BP (C)	BP (R)	BP (K)
8001	T-BUTYLACETYLENE	No	C6H10	82.14	99.90	37.72	559.57	310.87
8001	3,3-DIMETHYL-1-BUTYNE	No	C6H10	82.14	99.90	37.72	559.57	310.87
8002	2-ETHYL-1,3-BUTADIENE	No	C6H10	82.14	167.00	75.00	626.67	348.15
8003	1,2-HEXADIENE	No	C6H10	82.14	169.00	76.11	628.67	349.26
8003	PROPYLALLENE	No	C6H10	82.14	169.00	76.11	628.67	349.26
8004	1,CIS-3-HEXADIENE	No	C6H10	82.14	163.00	72.78	622.67	345.93
8005	1,TRANS-3-HEXADIENE	No	C6H10	82.14	163.00	72.78	622.67	345.93
8006	1,CIS-4-HEXADIENE	No	C6H10	82.14	149.00	65.00	608.67	338.15
8007	1,TRANS-4-HEXADIENE	No	C6H10	82.14	149.00	65.00	608.67	338.15
8008	2,3-HEXADIENE	No	C6H10	82.14	154.40	68.00	614.07	341.15
8009	CIS-2-CIS-4-HEXADIENE	No	C6H10	82.14	176.00	80.00	635.67	353.15
8010	CIS-2-TRANS-4-HEXADIENE	No	C6H10	82.14	176.00	80.00	635.67	353.15
8011	TRANS-2-TRANS-4-HEXADIENE	No	C6H10	82.14	176.00	80.00	635.67	353.15
8012	2-HEXYNE	No	C6H10	82.14	184.14	84.52	643.81	357.67
8012	METHYL PROPYLACETYLENE	No	C6H10	82.14	184.14	84.52	643.81	357.67
8013	2-METHYL-1,CIS-3-PENTADIENE	No	C6H10	82.14	169.00	76.11	628.67	349.26
8014	2-METHYL-1,TRANS-3-PENTADIENE	No	C6H10	82.14	169.00	76.11	628.67	349.26
8015	2-METHYL-1,4-PENTADIENE	No	C6H10	82.14	133.00	56.11	592.67	329.26

# Database Components

8016	2-METHYL-2,3-PENTADIENE	No	C6H10	82.14	162.00	72.22	621.67	345.37
8017	3-METHYL-1,2-PENTADIENE	No	C6H10	82.14	158.00	70.00	617.67	343.15
8018	3-METHYL-1,CIS-3-PENTADIENE	No	C6H10	82.14	171.00	77.22	630.67	350.37
8019	3-METHYL-1,TRANS-3-PENTADIENE	No	C6H10	82.14	171.00	77.22	630.67	350.37
8020	3-METHYL-1,4-PENTADIENE	No	C6H10	82.14	131.00	55.00	590.67	328.15
8021	ISOPROPYLALLENE	No	C6H10	82.14	158.00	70.00	617.67	343.15
8021	4-METHYL-1,2-PENTADIENE	No	C6H10	82.14	158.00	70.00	617.67	343.15
8022	4-METHYL-1,3-PENTADIENE	No	C6H10	82.14	169.30	76.28	628.97	349.43
8023	SEC-BUTYLACETYLENE	No	C6H10	82.14	135.90	57.72	595.57	330.87
8023	3-METHYL-1-PENTYNE	No	C6H10	82.14	135.90	57.72	595.57	330.87
8024	ISOBUTYLACETYLENE	No	C6H10	82.14	142.11	61.17	601.78	334.32
8024	4-METHYL-1-PENTYNE	No	C6H10	82.14	142.11	61.17	601.78	334.32
8025	METHYL ISOPROPYLACETYLENE	No	C6H10	82.14	163.63	73.13	623.30	346.28
8025	4-METHYL-2-PENTYNE	No	C6H10	82.14	163.63	73.13	623.30	346.28
8026	P-T-BUTYL TOLUENE	No	C11H16	148.25	378.97	192.76	838.64	465.91
8026	4-METHYL-1-BUTYLBENZENE	No	C11H16	148.25	378.97	192.76	838.64	465.91
8027	CHLOROACETONE	No	C3H5CLO	92.53	246.20	119.00	705.87	392.15
8027	1-CHLORO-2-PROPANONE	No	C3H5CLO	92.53	246.20	119.00	705.87	392.15
8028	DIPENTENE	No	C10H16	136.24	346.37	174.65	806.04	447.80
8028	LIMONENE	No	C10H16	136.24	346.37	174.65	806.04	447.80
8028	δ-P-MENTHA-1,8-DIENE	No	C10H16	136.24	346.37	174.65	806.04	447.80
8029	ACETYLKETENE	No	C4H4O2	84.07	260.60	127.00	720.27	400.15
8029	DIKETENE	No	C4H4O2	84.07	260.60	127.00	720.27	400.15
8029	VINYLACETO-β-LACTONE	No	C4H4O2	84.07	260.60	127.00	720.27	400.15
8030	2-CHLOROTOLUENE	No	C7H7CL	126.58	318.47	159.15	778.14	432.30
8030	O-CHLOROTOLUENE	No	C7H7CL	126.58	318.47	159.15	778.14	432.30
8031	4-CHLOROTOLUENE	No	C7H7CL	126.58	324.32	162.40	783.99	435.55
8031	P-CHLOROTOLUENE	No	C7H7CL	126.58	324.32	162.40	783.99	435.55
8032	3,4-DICHLOROTOLUENE	No	C7H6CL2	161.03	408.06	208.92	867.73	482.07
8033	METHYL ACETOACETATE	No	C5H8O3	116.11	337.10	169.50	796.77	442.65
8033	METHYL 3-OXOBUTANOATE	No	C5H8O3	116.11	337.10	169.50	796.77	442.65
8034	ACETAMIDE	No	C2H5NO	59.07	430.07	221.15	889.74	494.30
8034	ETHANEAMIDE	No	C2H5NO	59.07	430.07	221.15	889.74	494.30
8035	BENZAL CHLORIDE	No	C7H6CL2	161.03	401.36	205.20	861.03	478.35
8035	BENZYLIDENE CHLORIDE	No	C7H6CL2	161.03	401.36	205.20	861.03	478.35
8035	(1,1-DICHLOROMETHYL)BENZENE	No	C7H6CL2	161.03	401.36	205.20	861.03	478.35
8035	α-DICHLOROTOLUENE	No	C7H6CL2	161.03	401.36	205.20	861.03	478.35
8036	T-BUTYL ACETATE	No	C6H12O2	116.16	207.50	97.50	667.17	370.65
8036	T-BUTYL ETHANOATE	No	C6H12O2	116.16	207.50	97.50	667.17	370.65
8037	DI-T-BUTYL PEROXIDE	No	C8H18O2	146.22	225.41	107.45	685.08	380.60
8038	1-AMINO-2-PROPANOL	No	C3H9NO	75.11	319.03	159.46	778.70	432.61
8038	ISOPROPANOLAMINE	No	C3H9NO	75.11	319.03	159.46	778.70	432.61
8039	3-CHLORO-2-METHYL-1-PROPENE	No	C4H7CL	90.55	161.96	72.20	621.63	345.35
8039	METHALLYL CHLORIDE	No	C4H7CL	90.55	161.96	72.20	621.63	345.35
8040	3,5-DIMETHYL-1-HEXANOL	No	C8H18O	130.22	361.40	183.00	821.07	456.15
8041	ISOXAZOLE	No	C3H3NO	69.06	203.45	95.25	663.12	368.40
8042	DIPHENYL AMINE	No	C12H11N	169.23	575.60	302.00	1035.27	575.15
8042	N-PHENYLANILINE	No	C12H11N	169.23	575.60	302.00	1035.27	575.15
8043	INDENE	No	C9H8	116.16	358.97	181.65	818.64	454.80
8043	INDONAPHTHALENE	No	C9H8	116.16	358.97	181.65	818.64	454.80
8044	2,2-DIMETHYLPROPANOIC ACID	No	C5H10O2	102.13	326.63	163.68	786.30	436.83
8044	α-DIMETHYLPROPIOIC ACID	No	C5H10O2	102.13	326.63	163.68	786.30	436.83
8044	NEOPENTANOIC ACID	No	C5H10O2	102.13	326.63	163.68	786.30	436.83
8044	PIVALIC ACID	No	C5H10O2	102.13	326.63	163.68	786.30	436.83
8044	TRIMETHYLACETIC ACID	No	C5H10O2	102.13	326.63	163.68	786.30	436.83
8045	2-HYDROXY-1-ISOPROPYL-4-METHYL-BENZENE	No	C10H14O	150.22	449.33	231.85	909.00	505.00
8045	5-METHYL-2-ISOPROPYLPHENOL	No	C10H14O	150.22	449.33	231.85	909.00	505.00
8045	THYMOL	No	C10H14O	150.22	449.33	231.85	909.00	505.00
8046	1,2,4-TRICHLOROENZENE	No	C6H3CL3	181.45	415.49	213.05	875.16	486.20
8047	1,3-DIVINYLBENZENE	No	C10H10	130.20	391.19	199.55	850.86	472.70
8047	M-DIVINYLBENZENE	No	C10H10	130.20	391.19	199.55	850.86	472.70
8048	2-DECANOL	No	C10H22O	158.29	422.63	217.02	882.30	490.17
8049	METHACRYLONITRILE	No	C4H5N	67.09	194.53	90.29	654.20	363.44
8049	2-METHYL-2-PROPENONITRILE	No	C4H5N	67.09	194.53	90.29	654.20	363.44
8050	2,4,4-TRIMETHYL-2-PENTANOL	No	C8H18O	130.23	297.33	147.41	757.00	420.56
8051	TRANS-(2-CHLOROETHENYL)-BENZENE	No	C8H7CL	138.60	390.20	199.00	849.87	472.15
8051	TRANS-β-CHLOROSTYRENE	No	C8H7CL	138.60	390.20	199.00	849.87	472.15
8051	VINYL BENZYL CHLORIDE	No	C8H7CL	138.60	390.20	199.00	849.87	472.15
8052	P-ANISALDEHYDE	No	C8H8O2	136.16	481.10	249.50	940.77	522.65
8052	4-METHOXYBENZALDEHYDE	No	C8H8O2	136.16	481.10	249.50	940.77	522.65

## Chapter 2

8053	M-ANISALDEHYDE	No	C8H8O2	136.16	446.00	230.00	905.67	503.15
8053	3-METHOXYBENZALDEHYDE	No	C8H8O2	136.16	446.00	230.00	905.67	503.15
8054	O-ANISIDINE	No	C7H9NO	123.16	435.20	224.00	894.87	497.15
8054	2-METHOXY-1-AMINOBENZENE	No	C7H9NO	123.16	435.20	224.00	894.87	497.15
8054	2-METHOXYANILINE	No	C7H9NO	123.16	435.20	224.00	894.87	497.15
8055	M-ANISIDINE	No	C7H9NO	123.16	483.83	251.02	943.50	524.17
8055	3-METHOXY-1-AMINOBENZENE	No	C7H9NO	123.16	483.83	251.02	943.50	524.17
8055	3-METHOXYANILINE	No	C7H9NO	123.16	483.83	251.02	943.50	524.17
8056	P-ANISIDINE	No	C7H9NO	123.16	469.43	243.02	929.10	516.17
8056	4-METHOXY-1-AMINOBENZENE	No	C7H9NO	123.16	469.43	243.02	929.10	516.17
8056	4-METHOXYANILINE	No	C7H9NO	123.16	469.43	243.02	929.10	516.17
8057	METHYLETHYLACETYLENYLCARBINOL	No	C6H10O	98.15	248.93	120.52	708.60	393.67
8057	METHYLPENTYNOL	No	C6H10O	98.15	248.93	120.52	708.60	393.67
8057	3-METHYL-1-PENTYN-3-OL	No	C6H10O	98.15	248.93	120.52	708.60	393.67
8058	1,3-DIISOPROPYLBENZENE	No	C12H18	162.28	397.73	203.18	857.40	476.33
8058	M-DIISOPROPYLBENZENE	No	C12H18	162.28	397.73	203.18	857.40	476.33
8059	1,2-DIISOPROPYLBENZENE	No	C12H18	162.28	398.75	203.75	858.42	476.90
8059	O-DIISOPROPYLBENZENE	No	C12H18	162.28	398.75	203.75	858.42	476.90
8060	CYCLOPENTADIENE	No	C5H6	66.10	108.50	42.50	568.17	315.65
8061	ETHYL 2-NITROPHENYL ETHER	No	C8H9NO3	167.17	512.63	267.02	972.30	540.17
8061	2-NITRO-1-ETHOXYBENZENE	No	C8H9NO3	167.17	512.63	267.02	972.30	540.17
8061	O-NITROPHENETOLE	No	C8H9NO3	167.17	512.63	267.02	972.30	540.17
8061	O-NITROPHENETHYL ALCOHOL	No	C8H9NO3	167.17	512.63	267.02	972.30	540.17
8062	ETHYL 3-NITROPHENYL ETHER	No	C8H9NO3	167.17	543.23	284.02	1002.90	557.17
8062	3-NITRO-1-ETHOXYBENZENE	No	C8H9NO3	167.17	543.23	284.02	1002.90	557.17
8062	M-NITROPHENETOLE	No	C8H9NO3	167.17	543.23	284.02	1002.90	557.17
8062	M-NITROPHENETHYL ALCOHOL	No	C8H9NO3	167.17	543.23	284.02	1002.90	557.17
8063	ETHYL 4-NITROPHENYL ETHER	No	C8H9NO3	167.17	541.43	283.02	1001.10	556.17
8063	4-NITRO-1-ETHOXYBENZENE	No	C8H9NO3	167.17	541.43	283.02	1001.10	556.17
8063	P-NITROPHENETOLE	No	C8H9NO3	167.17	541.43	283.02	1001.10	556.17
8063	P-NITROPHENETHYL ALCOHOL	No	C8H9NO3	167.17	541.43	283.02	1001.10	556.17
8064	2-ETHOXY-1-AMINOBENZENE	No	C8H11NO	137.18	450.53	232.52	910.20	505.67
8064	2-ETHOXYANILINE	No	C8H11NO	137.18	450.53	232.52	910.20	505.67
8064	O-PHENETIDINE	No	C8H11NO	137.18	450.53	232.52	910.20	505.67
8065	3-ETHOXY-1-AMINOBENZENE	No	C8H11NO	137.18	478.43	248.02	938.10	521.17
8065	3-ETHOXYANILINE	No	C8H11NO	137.18	478.43	248.02	938.10	521.17
8065	M-PHENETIDINE	No	C8H11NO	137.18	478.43	248.02	938.10	521.17
8066	4-ETHOXY-1-AMINOBENZENE	No	C8H11NO	137.18	479.46	248.59	939.13	521.74
8066	4-ETHOXYANILINE	No	C8H11NO	137.18	479.46	248.59	939.13	521.74
8066	P-PHENETIDINE	No	C8H11NO	137.18	479.46	248.59	939.13	521.74
8067	3-TOLUENECARBOXYLIC ACID	No	C8H8O2	136.16	505.43	263.02	965.10	536.17
8067	M-TOLUIC ACID	No	C8H8O2	136.16	505.43	263.02	965.10	536.17
8068	2-TOLUENECARBOXYLIC ACID	No	C8H8O2	136.16	498.23	259.02	957.90	532.17
8068	O-TOLUIC ACID	No	C8H8O2	136.16	498.23	259.02	957.90	532.17
8069	ISOPHORONE	No	C9H14O	138.21	419.36	215.20	879.03	488.35
8069	3,5,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE	No	C9H14O	138.21	419.36	215.20	879.03	488.35
8070	ADIPONITRILE	No	C6H8N2	108.15	563.03	295.02	1022.70	568.17
8070	1,6-HEXANEDINITRILE	No	C6H8N2	108.15	563.03	295.02	1022.70	568.17
8070	1,4-DICYANOBUTANE	No	C6H8N2	108.15	563.03	295.02	1022.70	568.17
8071	ETHYL PHENYL BENZYLAMINE	No	C15H17N	211.31	595.13	312.85	1054.80	586.00
8072	2-ETHYLPYRIDINE	No	C7H9N	107.16	299.53	148.63	759.20	421.78
8073	3-ETHYLPYRIDINE	No	C7H9N	107.16	329.03	165.02	788.70	438.17
8074	4-ETHYLPYRIDINE	No	C7H9N	107.16	333.83	167.68	793.50	440.83
8075	2-ETHYL-4-METHYLPYRIDINE	No	C8H11N	121.18	345.23	174.02	804.90	447.17
8076	SYM-COLLIDINE	No	C8H11N	121.18	338.93	170.52	798.60	443.67
8076	2,4,6-TRIMETHYLPYRIDINE	No	C8H11N	121.18	338.93	170.52	798.60	443.67
8076	2,4,6-COLLIDINE	No	C8H11N	121.18	338.93	170.52	798.60	443.67
8077	DIBUTYL AMINE	No	C8H19N	129.25	318.20	159.00	777.87	432.15

## Component Database - ID From 9000 to 9999

The components ID numbers between 9000-9005 in DESIGN II database have the name, structure, molecular weight, normal boiling point, liquid density, critical temperature, and critical pressure. For other properties see *Component Properties Estimation Methods*. The component ID numbers between 9005-9999 are DESIGN II Ionic component database and user defined ionic species.

DESIGN		Mixed		Molecular				
II ID	Name	Amine	Formula	Weight	BP (F)	BP (C)	BP (R)	BP (K)
9001	AMMONIUM CHLORIDE	No	NH4CL	53.50	642.93	339.41	1102.60	612.56
9002	COPPER ALUMINUM CHLORIDE	No	CUALCL4	232.36	642.93	339.41	1102.60	612.56

9003	SODIUM HYDROXIDE	No	NAOH	40.00	642.93	339.41	1102.60	612.56
9004	POTASSIUM HYDROXIDE	No	KOH	56.10	642.93	339.41	1102.60	612.56
9401	H+	No	H+					
9402	OH-	No	OH-					
9631	S=	No	S=					
9632	HS-	No	HS-					
9633	SO3=	No	SO3=					
9634	HSO3-	No	HSO3-					
9651	CO3=	No	CO3=					
9652	HCO3-	No	HCO3-					
9661	CN-	No	CN-					
9701	NH4+	No	NH4+					
9711	NH2COO-	No	NH2COO-					
9900	Ionic-9900	No						
9901	Ionic-9901	No						
9902	Ionic-9902	No						
9903	Ionic-9903	No						
9904	Ionic-9904	No						
9905	Ionic-9905	No						
9906	Ionic-9906	No						
9907	Ionic-9907	No						
9908	Ionic-9908	No						
9909	Ionic-9909	No						
9910	Ionic-9910	No						

## Component Database for Mixed Amine

Components available in Mixed Amine thermodynamics form a subset of the components listed in Reid, Prausnitz and Sherwood's "The Properties of Gases and Liquids", Third Edition, McGraw-Hill Book Co, NY, 1977.

Listed below are 47 components grouped for use along with the Amines (MEA, DEA, MDEA, DGA, and DIPA). Note that "Mixed Amine" method applies only to this set of components. If other components not in this list are present "Mixed Amine" thermodynamic approach will not be used.

<u>DESIGN II ID</u>	<u>Name</u>	<u>Formula</u>
1	HYDROGEN	H2
2	METHANE	CH4
3	ETHANE	C2H6
4	PROPANE	C3H8
5	ISOBUTANE; 2-METHYLPROPANE	C4H10
6	N-BUTANE	C4H10
7	ISOPENTANE	C5H12
8	N-PENTANE	C5H12
9	NEOPENTANE; 2,2-DIMETHYLPROPANE	C5H12
10	N-HEXANE	C6H14
11	N-HEPTANE	C7H16
22	ETHYLENE	C2H4
23	PROPYLENE; PROPENE	C3H6
24	1-BUTENE	C4H8
27	ISOBUTYLENE; 2-METHYLPROPENE	C4H8
28	1,3-BUTADIENE	C4H6
36	CYCLOPENTANE	C5H10
37	METHOCYCLOPENTANE	C6H12
38	CYCLOHEXANE	C6H12
39	METHYL CYCLOHEXANE	C7H14
40	BENZENE	C6H6
41	TOLUENE	C7H8
42	o-XYLENE	C8H10
43	m-XYLENE	C8H10
44	p-XYLENE	C8H10
45	ETHYL BENZENE	C8H10
46	NITROGEN	N2
47	OXYGEN	O2
48	CARBON MONOXIDE	CO
49	CARBON DIOXIDE	CO2
50	HYDROGEN SULFIDE	H2S
62	WATER	H2O
65	ACETYLENE	C2H2
66	METHYLACETYLENE; PROPYNE	C3H4
67	ETHYLACETYLENE; 1-BUTYNE	C4H6

1087	CARBONYL SULFIDE	COS
1156	CYCLOPROPANE; TRIMETHYLENE	C3H6
1159	ISOHEXANE; 2-METHYL PENTANE	C6H14
1171	ARGON	AR
1172	HELIUM	HE
1219	PIPERAZINE	C4H10N2
2053	DIGLYCOLAMINE; DGA	C4H11NO2
4051	DIETHANOLAMINE; DEA	C4H11NO2
4155	MONOETHANOLAMINE; MEA	C2H7NO
6012	DIISOPROPANOLAMINE; DIPA	C6H15NO2
7048	VINYLACETYLENE; 1-BUTEN-3-YNE	C4H4
7051	METHYLDIETHANOLAMINE; MDEA	C5H13NO2

The key factor limiting the number of compounds is the lack of solubility data in water.

Enter components into the components list and reference within DESIGN II by using either the component number or the component identifier.

**NOTE:**

1. Use of ChemTran is also not allowed when "Mixed Amine" thermodynamic method is selected.
2. The Henry's constants from neo-pentane are being used for 5 new components such as iso-pentane, n-pentane, n-hexane, n-heptane, and iso-hexane.

## Component Properties Stored

The DESIGN II *Database Components* contains the following physical properties for 886 chemicals:

molecular weight	characteristic volumes	vapor pressure
boiling point	solubility parameter	acentric factor
critical properties	heat of vaporization	density
ideal gas heat capacities		

This data is made available to ChemTran and DESIGN II when the component ID number is entered in the COMponents command of the GENeral section of the input file. The programs then automatically retrieve all physical properties for that chemical and use them as they are needed. To view the properties of any component please see *ChemTran: Using ChemTran to Output Component Physical Properties*. There may be some cases where substitutions for some of the DATA BASE properties are desired. This can be accomplished by using *ChemTran* to prepare a CHEMtran FILE. A property is altered by inserting the appropriate command into the input commands and identifying the chemical by its Design II ID number. Any references to a standard or DATA BASE component in the input commands are made with these ID numbers. Nonstandard components are referred to in the same way, but the ID number assigned is as indicated in Table A-1. In addition, Table A-1 shows the amount of experimental data stored for each component ID number.

Several precautions have been taken to ensure the reliability of the data stored in the DATA BASE. Checks are made on the absolute range for a particular property and any deviations are accounted for. Property data estimates are made from more than one technique and compared to check their reliability. In addition, the basic experimental data is collected from standard reference sources and checked against various correlations.

**TABLE A-1: Component ID Numbers And Data Stored**

Component Numbers	Minimum Experimental Data Stored
1-99	MIN, Cp, Tc, Pc, acentric factor, (w) or Vc, solubility parameter (d), MW
100-199	User-provided petroleum fraction data
200-299	User-provided nonstandard component data (liquid or vapor)
300-399	User-provided solid component data
400-999	Reserved for future use
1000-1999	MIN, Cp, Tc, Pc, Ps
2000-2999	MIN, Tc, Pc, Ps
3000-3999	MIN, Cp, Ps
4000-4999	MIN, Ps
5000-5999	MIN, Cp, Pc, Tc
6000-6999	MIN, Pc, Tc
7000-7999	MIN, Cp
8000-8999	MIN

where MIN = name, structure, molecular weight, normal boiling point, and liquid density  
 Cp = ideal gas heat capacity as a function of temperature  
 Tc = critical temperature  
 Pc = critical pressure  
 w = acentric factor  
 Vc = critical volume  
 d = solubility parameter



Ps = vapor pressure as a function of temperature in range at least from 200 to 760 mmHg

Missing property data for components 2000-8999 has been estimated from the available experimental data. Please see *Component Properties Estimation Methods* for a description of the correlations used.

## Component Properties Estimation Methods

Missing property data for components 2000-8999 has been estimated from the available experimental data. The estimation methods employed for each property are described below:

- Ideal Gas Heat Capacity** - If applicable, the Benson method is used to estimate ideal gas heat capacity from structure. If not, the Parr method is used.
- Critical Temperature and Pressure** - The Lydersen method is used to estimate Tc and Pc from the structure.
- Vapor Pressure** - Vapor pressure is estimated from a reduced correlation equation, i.e., fitted to the normal boiling point and the critical point.
- Critical Volume** - If no critical volume is stored, it is estimated from a correlation based on Tc, Pc, and a liquid density value.
- Heat of Vaporization** - Although heats of vaporization are not included in the required list of stored data, an experimental value is included for their correlation when available. If a value is not available, the Clausius-Clayperon equation and experimental vapor pressure data are used for their calculation. If the vapor pressure data do not exist, the reduced vapor pressure correlation is used for their estimation.
- Other Parameters** - Other derived parameters are calculated from the more fundamental data discussed above; (a) solubility parameter from heat of vaporization and liquid density, (b) acentric factor from vapor pressure, (c) characteristic volume from liquid density and critical temperature.

## DESIGN II Ionic Component Library

### Ionic Components

9401 - 9899 Design II Ionic library components  
9900 - 9999 User-defined ionic components

The user can provide IONic FORmula, IONic CHARge, ION NAME, LIBrary REAction and REAction STOichiometry, EQUilibrium constants, and Henry's constants in water for ionic components using the ChemTran program.

<u>Ion ID Number</u>	<u>Ion</u>
9401	H+
9402	OH-
9631	S=
9632	HS-
9633	SO3-
9634	HSO3-
9651	CO3=
9652	HC03-
9661	CN-
9701	NH4+
9711	NH2COO-

### Library Reactions for Ionic Compounds

1-99	User-defined reactions
100+	Design II provided Reactions

Users can define the REAction STOichiometry and the LIBrary REAction numbers under *ChemTran: Electrolyte (Ionic) Component Data Entry*.

### Ionic Reaction Library

<u>Ionic Reaction ID</u>	<u>Ionic Reaction</u>
101	H2O<-> H+ + OH-
102	CO2 + H2O <-> H+ + HCO3-
103	HCO3- <-> H+ + CO3=
104	H2S <-> H+ + HS-
105	HS- <-> H+ + S-
106	SO2 + H2O <-> H+ + HSO3-
107	HSO3- <-> H+ + SO3 =
108	HCN <-> H+ + CN-
109	NH3 + H2O <-> NH4+ + OH-
110	NH3 + HCO3- <-> NH2COO- + H2O

**NOTE:** These reactions may be combined to specify other reactions. E.g. NH3 + CO2 + H2O <-> NH4+ + HCO3-. This is a combination of reactions 102 + 109 - 101.

## Chapter 2

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All specified reactions must be independent reactions. Any reaction in the system should be a linear combination of these reactions.

# Chapter 3: Specifying Feed Streams

Feed streams composed of components from the DESIGN II PURE COMPONENT DATABASE, or components added to DESIGN II database with Chemtran, or of known petroleum fractions are defined in the GENERAL section. Feed stream definition requires a minimum of three specifications:

- Composition
- Flowrate

And ONE of the following:

- Temperature and Pressure (recommended-default)

OR

- Pressure and Vapor Fraction (predicts Temperature with a starting guess) \*

OR

- Temperature and Vapor Fraction (predicts Pressure with a starting guess) \*

**\*NOTE:** Vapor Fraction specification must be a feasible flash for the pure or mixture of components, otherwise simulation will be stopped with cause of errors.

If your simulation has more than one feed, each feed must be numbered uniquely. All required specifications must be entered for each feed.

## Real Feeds Command Details

### Real Feeds Input Section Identification

The GENERAL section of a DESIGN II input file must be distinct from other input sections; i.e. Title, Equipment Modules, etc. Therefore, this section is initialized with the following command:

#### GENERAL

Must be the first command in the GENERAL section. There can be more than one GENERAL section per DESIGN II run.

**Every input file must have a GENERAL section.**

### Real Feeds Composition Specification

#### Listing Components

All flowsheet stream components are entered with one COMponents command. Each component must have a unique identification number. ID numbers 1-98 and 1000-9899 are assigned in Design II and are in the *Database Components*. ID numbers 100-399 and 9900 - 9999 are user assigned component numbers. Ionic components require an IONic COMponents command.

ID Numbers	Component Type
1 - 99	Pure Component Database
100 - 199	User Provided Petroleum Fraction
200 - 299	User Provided Nonstandard
300 - 399	User Provided Solids
500 - 999	User Provided Petroleum Fraction
1000 - 9400	Pure Component Database
9401 - 9899	Pure Component Database (ionic)
9900 - 9999	User Provided Ionic Components

The following command is used to list the components for the simulation.

#### COMponents =

Enter the ID numbers for every component in the simulation. Separate each number with a comma. Multiple GENERAL sections are allowed per simulation but there can be **only one COMponents command per simulation. Every simulation must have a COMponents command.**

#### IONic COMponents =

Enter the ID numbers for all ionic components involved in your simulation, if any. This command is required with the EDWARDK thermodynamic option. Ionic formula and charge data information should be entered and is found in the *ChemTran: Electrolyte (Ionic) Component Data Entry* section.

#### LIBrary REACTIONS =

Enter the reaction numbers in which the ionic components are involved. This command is required with the EDWARDK thermodynamic option. Reaction must be defined and is found in the *ChemTran: Electrolyte (Ionic) Component Data Entry*.

#### Data Base Components

Design II identification numbers for more than 886 real components are given in the *Database Components*. Physical property data stored for each of these components is automatically accessed by DESIGN II when the component ID number is listed with the COMponents command. Simply enter the Design II ID number for each of the components in your process. Names for

## Chapter 3

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components contained in the *Database Components* are automatically printed in the final stream summaries.

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### Real Feeds Flowrate Specification

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Feed flowrates may be specified in one of three ways:

- Component by component
- Component fractions and a total stream flowrate
- Flowrate set equal to the flowrate of a stream already defined in the current GENERAL section

The commands to specify feed flowrates in these ways are, respectively:

**FLOWrate (Q units/t units) j =**

Enter the flowrate of each component separated by commas. The flowrates must be listed in the same order as the component ID numbers in the COM command. "j" is the stream number from your flowsheet. Even if a component is not contained in a stream, a flowrate of zero must be entered to maintain the proper order.

**FLOWrate (FRA) j = (default molar fraction) and**

**TOTAL FLOW (Q units/t units) j =**

Use the FRAction option to enter mass, molar, or volume fractions for each component in the feed. If the FRActions do not total 1, they will be normalized. The fractions must be listed in the same order as the component ID numbers in the COM command. Even if a component is not contained in a stream, a flowrate of zero must be entered to maintain the proper order.

Use the TOT FLO command to enter the total flowrate for feed "j". The fraction units can be mixed and matched with the Q units on the TOTAl FLOW command. New fraction commands available for use are...

**FLOWrate (FRA MOL or FRA MAS or FRA VOL) j =**

**FLO x = FLO y**

For cases where one or more feed streams have the same composition and flowrates, you can set the flowrate of the second stream(s) equal to the flowrate of the defined stream. "x" is the stream which has identical flowrates and composition, "y" is the stream for which you have entered flowrates using one of the methods above.

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### Real Feeds Temperature, Pressure, and Vapor Fraction Specifications

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#### Temperature and Pressure Specification

The temperature and pressure must always be specified for each feed stream. These specifications are entered in the GENERAL section in one of two ways:

- Directly, by entering temperature and pressure values
- Indirectly, by setting the temperature and pressure of a feed equal to a stream previously defined in the GENERAL section. The commands to specify feed temperature and pressure in these ways are, respectively:

**TP (T units, P units) j =**

Enter the temperature and pressure, separated by a comma, for a feed stream; "j" is the stream number from your flowsheet. A temperature and pressure specification is always required.

**TP x = TP y**

For cases where one or more feed streams have the same temperature and pressure, you can set the temperature and pressure of the secondary stream(s) equal to that of a defined stream. "x" is the stream which has identical temperature and pressure, "y" is the stream for which you have entered temperature and pressure data using the method above.

#### Vapor Fraction Specification

**VAPor FRAction j = fraction, option**

Enter the vapor fraction and option, separated by a comma, for a feed stream; "j" is the stream number from your flowsheet. A temperature and pressure specification or guess is always required as per the option below.

Option\*:

- 1 - Specify Pressure and Vapor Fraction with a starting guess for Temperature. The resulting stream will show the predicted temperature for the given pressure and vapor fraction.
- 2 - Specify Temperature and Vapor Fraction with a starting guess for Pressure. The resulting stream will show the predicted pressure for the given temperature and vapor fraction.

**\*NOTE:** Vapor Fraction specification must be a feasible flash for the pure or mixture of components, otherwise simulation will be stopped with cause of errors.

## Real Feeds Command Summary

### Input Section Identification

**GENeral**

### Composition Specification

**COM**ponents =  
**AMB**(T units) **i** =  
**API**(G units) **i** =  
**AMW** **i** =  
**NAME** **i** =

### Flowrate Specification

**FLO**wrate (Q units/t units) **j** =  
**FLO**wrate (**FRA** - default in MOL or **FRA MOL** or  
**FRA MAS** or **FRA VOL**) **j** =  
*and*  
**TOT**al **FLO**wrate (Q units/t units) **j** =  
**FLO** **x** = **FLO** **y**

### Temperature and Pressure Specification

**TP** (T units, P units) **j** =  
**TP** **x** = **TP** **y**

### Vapor Fraction Specification

**VAP FRA** **j** =

### Stream Phase Specification

**LIQ**uid = **j**, ..  
**VAP**or = **j**, ..

## Real Feeds Stream Phase Specification

These commands are not normally required, since stream phase conditions are automatically determined by the program. In situations where the stream conditions are predicted incorrectly by the program (possibly above the phase envelope), the conditions can be specified with the phase commands. Intermediate streams that will be calculated by equipment modules cannot have their phase conditions set since they will be recalculated by the equipment module. The only streams that can be set are feed streams to the process.

DESIGN II automatically calculates whether a feed stream is all liquid, all vapor, or mixed phase. If a stream is to be at its bubble point or dew point condition, the preferred method is to use an appropriate module to calculate the condition. The HEAT EXChanger module can be used to calculate bubble or dew point temperatures at a given pressure; the VALve module can be used to calculate bubble or dew point pressures at a given temperature; the FLAsh and MULTiple FLAsh modules can be used for either calculation.

Use the following commands to set the phase of the feed stream:

**LIQ**uid = **j**, ...

This command forces feed stream number(s) "j", ... to be liquid. If more than one stream is to be specified as liquid, the other stream numbers would be listed in the same command.

**VAP**or = **j**, ...

This command forces feed stream number(s) "j", ... to be vapor. If more than one stream is to be specified as vapor, the other stream numbers would be coded on the same command.

## Real Feeds Heating Value Commands

### **Value Specification**

Added support for specifying Lower Heating Value and Higher Heating Value for all components. Previously could only add heating values for petroleum fractions. Also, Heating Values may be specified in quantity over mass dimensional units (i.e. btu/lb or btu/gal). If mass units are used for the dimensionl units then it is presumed that the fluid is in a liquid state and latent heat will be added to it.

The heating value calculated by DESIGN II for all components can also be adjusted by entering your own value for the CARbon to HYDrogen weight ratio for each component. You can also use these commands to enter heating values for

## Chapter 3

component in the **Pure Component Data Base**.

The methods used by DESIGN II to obtain heating values and carbon-to-hydrogen ratios are based on general correlations. Greater accuracy in the calculations can be obtained by using laboratory-derived high or low heating values or carbon/hydrogen ratios.

(choose any of the following options)

**HIGH HEATING** value (H units/molar Q units)

Enter desired high (wet) heating value for petroleum fraction "i", where "i" is the component ID number. High heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with liquid water formed by the reaction.

**LOW HEATING** value (H units/molar Q units) **i =**

Enter desired low heating value for petroleum fraction "i", where "i" is the component ID number. The low heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with water remaining in the gaseous state.

**CARBON to HYDROGEN** weight ratio **i =**

Enter the desired value for petroleum fraction "i", where "i" is the component ID number. The heating value calculated by DESIGN II for petroleum fraction components CARBON to HYDROGEN weight ratio for each petroleum fraction. The default value will be calculated using Figure 2B2.1 from the API *Technical Data Book*.

Be sure to enter at least four significant figures for the CAR HYD command as this value can affect the mass balance in reactor calculations.

### Petroleum (Pseudo) Fractions

Known petroleum fraction feed components may be listed in the GENERAL section. Each fraction requires the following information, at a minimum.

- An arbitrary, unique ID number from 100 to 199 and 500 to 999
- Mean Average Boiling Point
- An API gravity

Optionally, average molecular weight and a component name may be entered. If the molecular weight is not entered, it will be calculated as a function of the boiling point and gravity, using the CAVETT correlation. This correlation is reasonable for light crudes and most lean oils. Heavier and more aromatic crudes may require a different correlation. See *Petroleum Fractions Molecular Weight Estimation Options*. If a component name is not entered, the component will be identified by its specified boiling point.

### Petroleum Fraction Essential Commands

Use the following commands to enter data for petroleum fractions.

**AMB** (T units) **i =**

Enter the mean average boiling point of the petroleum fraction; "i" is the component ID number assigned to the fraction (between 100-199 and 500-999). This specification is required for all petroleum fractions.

**API** (G units) **i =**

Enter the gravity of the petroleum fraction; "i" is the component ID number. This specification is required for all petroleum fractions.

**AMW** **i =**

Enter the average molecular weight of the petroleum fraction; "i" is the component ID number. This specification is optional. If not entered, it will be estimated from AMB and API.

**NAME** **i =**

Use this command to enter your own name for a petroleum fraction or any other component you wish to name; "i" is the component ID number. The maximum is 16 characters per name. Do not use commas in the name. If no name is entered, the fraction will be identified by its specified boiling point.

**Remember** when you are using the AMB, API and AMW commands that you must assign each petroleum fraction a unique component ID number between 100-199 and 500-999. These numbers must be entered with the COMPOONENTS command.

**NOTE:** If you are using CRUDE feed commands to describe any feeds in your flowsheet, you **cannot** use the petroleum fraction commands.

## Petroleum Fraction Optional Commands

DESIGN II allows using the following commands when the simulation contains user defined **PET**roleum fractions.

### Petroleum Fraction Critical Temperature Estimation Options

#### **DATa TC KEy =**

Enter option for prediction of critical temperature for petroleum fractions. Default option is **CAVett**. (choose one of the following options)

#### **CAVett**

This is the default correlation for calculating critical temperatures for petroleum fractions. Reference 44.

#### **COAL** liquids

Correlation developed by Wilson, et.al for estimating critical temperatures for petroleum fractions, especially those with Watson characterization factors which are less than 11. Reference 43.

#### **LEE**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions. References 25 and 31.

#### **NOKay**

Method for calculating critical pressure for paraffinic, olefinic, naphthenic and aromatic hydrocarbons with boiling points in the range of -40 to 1000F and specific gravities in the range of 0.5 to 1.0. Reference 45.

#### **WATson**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31, and 43.

### Petroleum Fraction Critical Pressure Estimation Options

#### **DATa PC KEy =**

Enter option for prediction of critical pressure for petroleum fractions. Default option is **CAVett**. (choose one of the following options)

#### **CAVett**

This is the default correlation for calculating critical pressures for petroleum fractions. Reference 44.

#### **COAL** liquids

Correlation developed by Wilson, et.al. for calculating critical pressures for petroleum fractions, especially those with Watson characterization factors which are less than 11. References 43.

#### **HERZog**

Method for estimating critical pressure using vapor pressure, boiling points and parachors for substances. Works best for saturated and unsaturated hydrocarbons; accuracy decreases for aromatic and cyclic compounds. Reference 46.

#### **LEE**

Lee-Kesler technique is used to calculate critical pressures for petroleum fractions. References 25 and 31.

#### **WATson**

The Lee-Kesler correlation is used to calculate critical pressures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31 and 43.

### Petroleum Fraction Molecular Weight Estimation Options

#### **DATa MOL KEy =**

Enter option for prediction of molecular weight for petroleum fractions. Default option for petroleum fractions entered in **GENeral** section is **CAVett**. Default option for **CRUDe** feed description is **HARiu**. (choose one of the following options).

#### **CAVett**

This is the default option for predicting molecular weight when petroleum fraction commands are entered in the **GENeral** section (AMB i =, API i =). Reference 44.

#### **API**

Technique developed by M. Riazi at the Pennsylvania State University for calculating molecular weights of petroleum fractions. This technique should be avoided for light hydrocarbons (hexanes and lighter). Reference 48.

#### **HARiu**

This is the default option for predicting molecular weights for petroleum fractions if you use any of the following in your simulation: **REFine** module, **CRUDe** feed section or **PETroleum STReam** print option. Reference 47.

#### **LEE**

Lee-Kesler correlation for calculating molecular weights for petroleum fractions. Reference 25 and 31.

### Petroleum Fraction Acentric Factor Estimation Options

At any time, additional thermophysical data for a particular component may be provided directly to DESIGN II for simulation calculation. The provided data will be used rather than allowing DESIGN II to estimate properties for the components

## Chapter 3

specified. The acentric factors (ACE) may be entered in the GENeral section of DESIGN II input. DESIGN II will use this data in subsequent calculations. The commands for entering this information are:

**ACE i =**

Enter acentric factor for component "i". Default method is Edmister. For additional command options see *ChemTran: Acentric Factor*.

### Petroleum Fractions Heating Value Specification

You can override the default heating value which DESIGN II will calculate for the petroleum fraction components by entering a HIGH HEATING value or LOW HEATING value command for each petroleum fraction. The heating value calculated by DESIGN II for petroleum fraction components can also be adjusted by entering your own value for the CARbon to HYDrogen weight ratio for each petroleum fraction. You can also use these commands to enter heating values for component in the Pure Component Data Base

The methods used by DESIGN II to obtain heating values and carbon-to-hydrogen ratios are based on general correlations. Greater accuracy in the calculations can be obtained by using laboratory-derived high or low heating values or carbon/hydrogen ratios. (choose any of the following options)

**HIGH HEATING** value (H units/molar Q units)

Enter desired high (wet) heating value for petroleum fraction "i", where "i" is the component ID number. High heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with liquid water formed by the reaction.

**LOW HEATING** value (H units/molar Q units) **i =**

Enter desired low heating value for petroleum fraction "i", where "i" is the component ID number. The low heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with water remaining in the gaseous state.

**CARBON to HYDROGEN** weight ratio **i =**

Enter the desired value for petroleum fraction "i", where "i" is the component ID number. The heating value calculated by DESIGN II for petroleum fraction components CARbon to HYDrogen weight ratio for each petroleum fraction. The default value will be calculated using Figure 2B2.1 from the API *Technical Data Book*. Be sure to enter at least four significant figures for the CAR HYD command as this value can affect the mass balance in reactor calculations.

### Feeds Thermodynamic Optional Command

Use these commands to specify individual feed (or recycle) streams thermodynamic methods, only when it is preferred to be different than the system **thermodynamic methods** specified in the GENeral commands (Specify...Basic Thermo). Additional keywords for different methods are given in the Thermodynamics Section. Also see Equipment Modules Thermodynamic Optional Command section.

**THErmo STRream KKEY i =**

Enter symbolic name for stream K-value option. (e.g. **THE STR KKEY i = PENK**)

**THErmo STRream HKEY i =**

Enter symbolic name for stream enthalpy option. (e.g. **THE STR HKEY i = ASOA**)

**THErmo STRream DKEY i =**

Enter symbolic name for stream density option. (e.g. **THE STR DKEY i = SOAV**)

**THErmo STRream LIQ DKEY i =**

Enter symbolic name for stream density option. (e.g. **THE STR LIQ DKEY i = PEND**)

**THErmo STRream TRANS i =**

Enter symbolic name for stream transport property option. (e.g. **THE STR TRANS i = API**)

**THErmo STRream VLKEY i =**

Enter symbolic name for stream liquid viscosity option. (e.g. **THE STR VLKEY i = LNAV**)

**THErmo STRream VVKEY i =**

Enter symbolic name for stream vapor viscosity option. (e.g. **THE STR VVKEY i = DEAN**)

**THErmo STRream TLKEY i =**

Enter symbolic name for stream liquid thermal conductivity option. (e.g. **THE STR TLKEY i = LI**)

**THErmo STRream TVKEY i =**

Enter symbolic name for stream vapor thermal conductivity option. (e.g. **THE STR TVKEY i = DEAN**)

**THErmo STRream STKEY i =**

Enter symbolic name for stream surface tension option. (e.g. **THE STR STKEY i = LI**)

**THErmo STRream IMMKEY i = ON (or OFF)**

Enter option for stream water immiscibility criteria. (e.g. **THE STR IMMKEY i = ON**)



## Specifying and Referencing a Feed Stream

### Specifying a Feed Stream

Given the following information for three feed streams, code the GENeral section input defining the feeds for a DESIGN II simulation .

#### Design II

Component Name	Component ID number	Feed 1 lb/hr	Feed 2 mol frac	Feed 3 lb/hr
Hydrogen	1	10	0.1	10
Methane	2	20	0.1	20
Ethane	3	30	0	30
Lean Oil (user assigned)	100	100	0.8	100
Temperature		10 F	10 F	70 C
Pressure		350 PSIA	350 PSIA	10 ATM
Total flowrate			500 lbmol/hr	

Average boiling point Lean Oil = 150 C  
Specific gravity Lean Oil = 0.70

### Referencing a Feed Stream

The user can also specify a feed stream with the results of a reference stream at calculation time. The commands to use reference streams is as follows:

**REF**erence **ST**ream  $x = y$

This command will specify any given feed stream with the results of a reference stream at calculation time. The Reference Stream's Results will be copied after the reference stream's equipment is executed. If the automatic unit module calculation sequence is turned on (by default), then the unit module that the feed stream is connected to will be placed after the unit module that calculates the reference stream.

### Specifying Feed STEP 1

**Initialize GENeral section ALWAYS REQUIRED.** Identify feed section type.

Section identifier GEN

### Specifying Feed STEP 2

**Assign all components ID numbers. List all components in input file with the COM = command - ALWAYS REQUIRED.** Identify ALL components in the process.

- Assign all known components an ID number by the following convention.

ID NUMBERS	COMPONENT TYPE
1 - 99	DATABASE (see <i>Component Database - ID From 1 to 99</i> )
100 - 199	USER PROVIDED PETROLEUM FRACTION
200 - 299	USER PROVIDED NON-STANDARD
300 - 399	USER PROVIDED SOLIDS
500 - 999	USER PROVIDED PETROLEUM FRACTION (continued)
1000 - 9999	DATABASE (see <i>Component Database Sorted By ID</i> )

Component ID numbers, separated by commas, for all components in the flowsheet COM =

### Specifying Feed STEP 3

**Characterize petroleum fractions by entering the data at right for EACH fraction. A component number from 100 - 199, a boiling point, and a gravity are the minimum required entries.** IF petroleum fractions THEN characterize by entering ALL of the following.

Each fraction must have a unique component ID # from 100 - 199. Substitute this number for *i* in the commands below

Average boiling point of the fraction AMB (T units) *i* =  
Gravity of the fraction @ 60 F API (G units) *i* =

## Chapter 3

---

IF molecular weight of fraction is known THEN

Average molecular weight of the fraction (if not entered, it is estimated from AMB and API) **AMW i =**

IF you wish to name the fraction THEN

Enter up to 16 characters (do not include commas). If no name is entered, the fraction will be identified by its specified boiling point **NAME i =**

---

### Specifying Feed STEP 4

---

**Feed flowrates are specified in one of three ways: 1) component flows 2) component fractions and total flows 3) set feed equal to a defined stream feed. A flowrate command IS ALWAYS REQUIRED.**

IF flowrate is on a component by component basis THEN

Flow of each component, separated by commas, in the same order as the components are listed in the COM = command for every feed stream "j" **FLO (Q units/t units) j =**

IF flowrate is on a fraction of total flow basis THEN enter BOTH of the following

Fraction of each component, separated by commas, in the same order as the components are listed in the COM command for every feed stream "j". If the sum of the values entered as fractions does not total 1.0, the values will be normalized **FLO (FRA) j =**

Total flow for feed "j". The Q units for the total flow must match the fractional units basis used in the FRA command **TOT FLO (Q units/t units) j =**

IF one or more streams have the same composition and flowrate THEN

Set the second stream equal to a stream defined by one of the above two methods. "x" is the stream that has identical composition and flowrate and "y" is the stream already defined **FLO x = FLO y**

---

### Specifying Feed STEP 5

---

**Enter temperature and pressure in one of two ways: 1) directly 2) equal to a previously defined stream A TP= command is ALWAYS REQUIRED.**

Feed stream temperature and pressure.

Temperature and pressure, separated by commas, of each feed stream "j" **TP (T units, P units) j =**

IF one or more streams have the same temperature and pressure THEN

Set the second stream equal to a stream whose T and P is defined by the above method. "x" is the stream that has identical T and P and "y" is the stream already defined **TP x = TP y**

Feed Vapor Fraction

Enter the vapor fraction and option, separated by a comma, for a feed stream; "j" is the stream number from your flowsheet. A temperature and pressure specification or guess is Always required as per the option below. **VAP FRA j =**  
Value, option

Option\*:

- 1 - Specify Pressure and Vapor Fraction with a starting guess for Temperature. The resulting stream will show the predicted temperature for the given pressure and vapor fraction.
- 2 - Specify Temperature and Vapor Fraction with a starting guess for Pressure. The resulting stream will show the predicted pressure for the given temperature and vapor fraction.

**\*NOTE:** Vapor Fraction specification must be a feasible flash for the pure or mixture of components, otherwise simulation will be stopped with cause of errors.

---

### Specifying Feed Example Coding

---

GENeral

```
AMB (C)100 = 150, API (SPG) = .70, NAME 100 = LEAN OIL
COMPONENTS = 1,2,3,100
FLOW (LB/HR) 1 = 10,20,30,100
FLOW (FRA) 2 = .10, .10, 0.0, .80, TOTAL FLOW 2 = 500
FLOW 3 = FLOW 1
TP 1 = 10, 350
TP 2 = TP 1
TP 3 (C, ATM) = 70, 10
```

# Chapter 4: Crude Bulk Feed Streams

The commands in the CRUde section describe hydrocarbon feeds, which are typically characterized by TBP or ASTM distillation curves. DESIGN II allows entry of as much information as you have for your feed(s) using simple keyword commands, from the minimum (distillation curve, bulk gravity, and feed rate) required to define a feed to additional data such as sulfur weight percent curves, viscosity curves, pour point, metals content, and more.

For each feed described by bulk properties in the CRUde section, the following are required:

- Composition (ASTM or TBP distillation curve)
- Bulk Gravity, Gravity Curve, or UOP K Factor
- Flowrate
- Temperature and Pressure
- Up to 200 Crude Feeds (includes recycle stream specifications) are allowed to be defined/specified for each flowsheet execution (single or linked).

If your simulation has more than one feed (should not exceed 200), each feed must be numbered uniquely. All required specifications must be entered for each feed.

---

## Crude Bulk Feed Command Details

---

### Crude Bulk Feed Input Section Identification

---

The CRUde section of a DESIGN II input file must be distinct from other input sections, e.g., Title, Equipment Modules, etc. Therefore, you must initialize this section with the following command.

#### CRUde

Must be the first command in the CRUde section.

---

### Crude Bulk Feed Blending

---

By default, all crude bulk feed streams and crude bulk recycle streams defined as crude cut curve (TBP or ASTM) will be characterized onto a single range of petroleum fractions. The petroleum fraction ranges used are: 101-199 and 500-999.

Users can make use of the following command to control the characterization (gravity, average boiling cut points, molecular weight, etc...) of all the different crude oil feed curves used within a simulation. This allows given properties to be maintained for each defined crude oil cut curve distribution (TBP or ASTM) without the back-blending discussed at [Crude Bulk Feed Back Blending Products to Recreate a Feed](#).

#### FEEd BLEND x = y

Enter this command to obtain uniform cut curve properties for each defined crude oil curve distribution. Here 'x' is the stream number and 'y' is the blend number. The program allows for up to 200 partially blended feeds.

#### Notes:

1. FEEd BLEnd must be the first command for each feed crude curve stream.
  2. Every feed to be blended with stream x will have the same blend number y (default is 1. Allowable blend number range is 1 to 200).
  3. If the blend command is used, a unique blend number must be given for every feed crude cut curve (TBP or ASTM) defined on the flowsheet.
  4. If streams are not blended with other streams, the command would still be given with the next available blend number. The blend numbers are in sequence beginning with 1 but later feeds blended with an earlier feed would repeat that number. For example, if the first stream uses blend 1 as in FEEd BLEND x1 = 1 and any later stream to be blended with it would also be FEEd BLEND x2 = 1. Here x1 and x2 are two stream numbers with same defined crude curve distribution. Other feed crude curve streams can be given using the same or different blend numbers, depending on user requirements on assay results.
- 

### Crude Bulk Feed Composition Specifications

---

## Chapter 4

### Real Components And Pseudocomponents

A distillation curve can be divided into two major portions: light-ends (real components) and pseudocomponents, as shown in Figure 1.

Since light ends consist of identifiable chemical compounds (ethane, butanes, etc.), whose properties are contained in the PURE COMPONENT DATA BASE, they are called real components. After allowing for the real components, DESIGN II automatically divides the rest of the distillation curve into "pseudocomponents".

Each real component and each pseudocomponent must have its own boiling point, flowrate, average gravity, and molecular weight. The following paragraphs explain how each portion is handled.

#### Light Ends Analysis For Bulk Feeds

Light ends (real components) can have a major impact on column behavior. Always provide this data if you have it or can get it. Two commands are used to enter a light-ends analysis: COM and FEE REAL j. Each command must appear in the proper input section to correctly specify a light ends analysis. Details of these commands appear below.

The COMponents = command must appear in the GENERAL section of the input file.

**COM**ponents = 62, .....

Enter component ID numbers from the *Database Components* separated by commas for all real components. Only one COMponents command is used to list real components for ALL feeds in an input, regardless of the number.

Water (ID=62) **must be the first component** listed in the COM command.

List remaining real components in order of ascending boiling point. Properties contained in the *Database Components* are automatically used for calculations.

Water must be the first component in the GENERAL section COMponents command. You should also specify IMM=62 in the GENERAL section if you are not using a K-value option which automatically treats water as immiscible.

The FEE REAL j = command belongs in the CRUDE section of the input file.

**FEE** REAL j =

Enter individual volume or weight percent (on a dry basis) for real components, separated by commas, in the order they appear in the COMponents command. Entries are assumed to be volume percents if a FEE VOLUME command is also entered, or weight percents if a FEE WEIGHT command is entered. "j" is the stream number. Do not include a value for water in this command. Each feed stream may have its own FEE REAL command, although only one COMponents command may be used.

Use of the FEE REAL command increases the accuracy with which the program calculates the effect of light ends. If you have listed real components in the COMponents command, but do not use the FEE REAL command, the program will account for the light portion of the curve as real rather than pseudocomponents. The light ends composition implied by the distillation curve is not as accurate as a true light ends analysis.

**Warning:** If you add a heavy component (EG, DEG, etc...) to a flowsheet with a crude section then the crude cuts will allocate most of any crude feed to the respective pure component (due to its high boiling point). Please note that the only component that the crude section automatic light end analysis ignores is water. Therefore, if and when you add light end components and heavies to the component list, please provide their individual feed quantity, so that the FEE REAL command becomes active for that feed stream. If light ends and heavy feed rates are absent (no FEE REAL command), the program will account for the light portion of the curve as real rather than pseudocomponents.

**NOTE:** DESIGN II does not account for the cooling effects caused by thermal cracking. Check for cracking by reviewing the column tray temperatures. Refer to API Figure 3A1.1 for data to use in making adjustments by adding light-end components to your feed. Use the two commands described above to enter any additional light ends.

#### Entering Distillation Curves

The most important aspect of entering a distillation curve is making sure that the shape of the curve accurately reflects the composition of the actual feed. You will have to use your own judgment in analyzing and adjusting your curve before making a rigorous run. In general, more distillation points rather than fewer give a more accurate composition.

Additionally, extra points in the 0-10% and 90-100% portion of the curve are more important than those in the flatter (30-70%) portion of the curve.

DESIGN II accepts TBP, ASTM D-86, ASTM D-1160 (760 mm), and ASTM D-1160 (10 mm) distillation curves. ASTM curves are automatically converted to TBP curves for use in program calculations. A maximum of 75 temperature values are allowed for each additional curve.

**NOTE:**

1. Multiple crude feed streams should have a minimum of 40 or so cut points defined for the entire crude range. This will provide good estimates of bulk gravity, and cut widths.

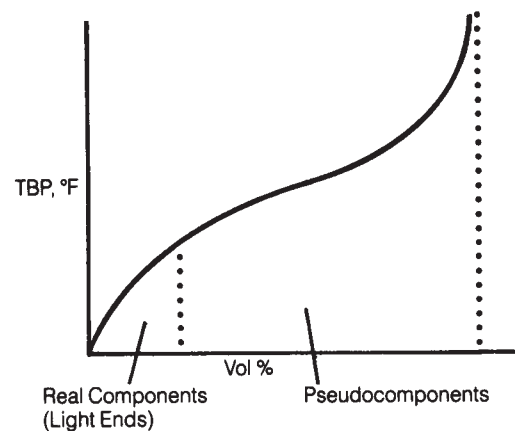


Figure 1. Real Components and Pseudocomponents

2. If the stream is a RECYCLE stream then crude properties are not to be specified.

For each feed defined by a distillation curve enter both the boiling-point temperature and the cumulative volume or weight percent corresponding to each temperature. Temperatures are entered using one of the following commands:

**FEEd ASTm T (units) j =**

Enter ASTM D-86 distillation temperatures, separated by commas, corresponding to the volume percents entered on the FEEd VOLume command, where "j" is the stream number.

**FEEd ASTm HIGH (T units) j =**

Enter ASTM D-1160 (760mm) distillation temperatures, separated by commas, corresponding to volume percents entered on the FEEd VOLume command, where "j" is the stream number.

**FEEd ASTm LOW (T units) j =**

Enter ASTM D-1160 (10 mm) distillation temperatures, separated by commas, corresponding to volume percents entered on the FEEd VOLume command, where "j" is the stream number.

**FEEd TBP (T units) j =**

Enter true boiling points, separated by commas, corresponding to volume percents entered on the FEEd VOLume command, where "j" is the stream number. The cumulative volume percents corresponding to the temperature values are entered using the FEEd VOLume percents command.

**FEEd TBPSD (T units) j =**

Enter true boiling points from a simulated distillation, separated by commas, corresponding to ONLY weight percents entered via the FEEd WEIght command, where "j" is the stream number. The cumulative weight percents corresponding to the temperature values are entered using the FEEd WEIght percents j = ... command shown below. Note that FEEd WEIght percents j = ...command should always precede this command on an input file.

**FEEd VOLume percents j =**

Enter the volume percents, separated by commas, at which the distillation temperatures were measured for stream number "j". If this command is not entered, default volume percents are assumed.

They are 0, 5, 10, 20, 30,40, 50, 60, 70, 80, 90, 95, 100.

Alternately, specify corresponding weight percents instead of volume percents using the FEEd WEIght percents command.

**FEEd WEIght percents j =**

Enter the weight percents, separated by commas, at which the distillation temperatures were measured for stream "j".

When you enter a FEE WEI command, all FEEd REAl commands, FEE GRA VOL commands, and FEE MOL VOL commands revert to a weight percent basis for that feed.

If you use the FEE WEI i command for a feed, all "FEEd" commands for that feed will be on a weight basis.

**Pseudocomponent Generation and Adjustment**

After removing the specified volume percents of any real components you have entered, DESIGN II automatically divides the rest of your distillation curve into pseudocomponents, assigning each a boiling point, flowrate, average gravity and molecular weight. The number and increments of the temperature cuts used to identify pseudocomponents depends on the range of the TBP values as described in Figures 2 and 3 below.

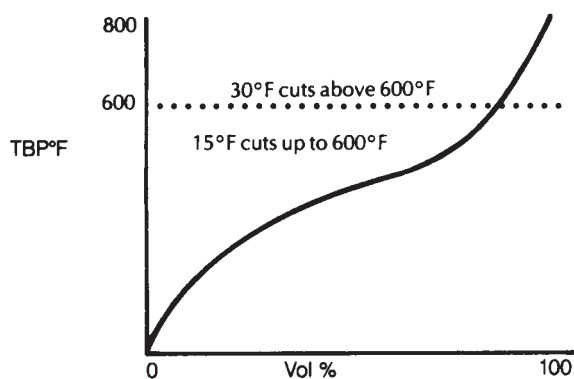


Figure 2. TBP less than 1,000 °F

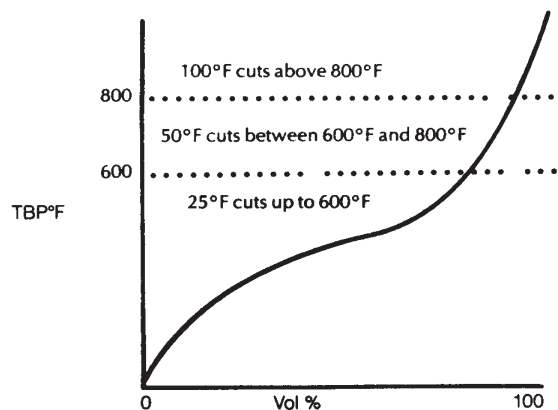


Figure 3. TBP higher than 1,000 °F

In many cases, you will find it necessary to make adjustments to the pseudocomponent slate generated by DESIGN II. For example:

- Too many pseudocomponents might be created.
- You might want more cuts in the mid-volume part of the feed and less in the heavy ends.

The number of cuts is very important for an adequate feed description. Too few cuts or very wide cuts make it difficult to calculate clear product distillation curves. It is recommended that each product contain about seven pseudocomponents (count light ends as one component when counting for the overhead liquid product).

There are two ways to alter the default pseudocomponent slate. First you may specify individual boiling point cuts directly

## Chapter 4

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using the CUT points command. If you do this, specify values covering the entire feed from initial boiling point to end point. You may also want to enter this command if the 95-100% portion of your distillation curve exceeds 1700F. In this case, the final temperature entered should not exceed 1800 F.

**CUT** points (T units) =

Enter mean average boiling points for all pseudocomponents in ascending order. The complete feed must be covered, from initial boiling point to end point. Only one CUT points command is allowed per run.

**NOTE:** Same command can be used to fix the starting CUT point when either default crude curve cuts are determined (or) when TEMperature BREak points and TEMperature INCrement values are being used.

Along with the CUT points command, you can change the DESIGN II default parameters for determining pseudocomponents. There are two parameters that you may control. These are the temperature break points and the temperature increments used between these breakpoints (See Figures 2 and 3). These parameters work together in setting cut sizes in DESIGN II. You may specify two TEMperature BREak points and three TEMperature INCrement values. Cut size is set by INCrement 1 up to BREak point 1, by INCrement 2 up to BREak point 2, and by INCrement 3 above BREak point 2.

Use the command below to set the temperature break points:

**TEM**perature of **BRE**aks (T units) =

Use this command to change the default temperature breaks for the initial to middle and middle to last temperature breakpoints. Defaults are 600F and 800 F. Enter two new values separated by commas.

You can also change the default cut sizes with the TEMperature of INCrements command. To change the default cut sizes enter:

**TEM**perature of **INC**rements (T units) =

Enter three values, separated by commas, to replace the default values of the temperature increments. Defaults: Initial section cut increment as 15 F or 25 F (when FBP > 1000 F); middle section cut increment as 35 F or 50 F (when FBP > 1000 F); final section cut increment as 100 F

**NOTE:** It is always a good idea to run a feed flash after you have made the adjustments to make sure the resulting cut increments are what you intended, from the starting cut point to the end point.

---

### Crude Bulk Feed Gravity Specifications

---

A gravity specification is always required in addition to the distillation curve. Whenever possible, you should enter a feed gravity versus volume percent curve. However, you can simply enter a whole feed gravity. If you do, DESIGN II calculates the gravity of each pseudocomponent as though it has the same UOP K as the whole feed.

To enter a gravity curve, use the commands below.

**FEEd GRA**vy (G units) **j** =

Enter gravity data, separated by commas, corresponding to the volume percents from the gravity curve.

**FEEd GRA**vy **VOL**ume percents **j** =

Enter volume percents, separated by commas, corresponding to gravity data entered on the FEEd GRAvy command. If this command is not entered, FEEd GRAvy values are assumed to correspond to the FEEd VOLume percents.

If a FEEd WEIght percents command was entered, the values entered here must be on a weight basis also.

**FEEd BULK GRA**vy (G units) **j** =

Optionally, enter the bulk feed gravity for stream number "j". Use this command only when you also enter gravities versus volume percents.

If you enter a gravity curve for a feed, you should also enter a bulk feed gravity with the FEEd BULK GRAvy j command. This entry is not required, but it results in a more realistic gravity curve. DESIGN II will adjust gravities of all pseudocomponents to meet the bulk gravity value.

Instead of entering a gravity curve, you can simply enter the whole feed gravity. To do this, you use the same FEEd GRAvy j command, but enter only a single value instead of a range of values.

**Example:** **FEE GRA** 10 = 33.7

Or, if you wish, enter one UOP characterization factor for each feed, instead of the whole gravity.

**FEEd UOP** j =

Enter one UOP characterization factor for feed stream "j" instead of the gravity.

**Example:** **FEE UOP** 10 = 12.06

---

### Crude Bulk Feed Flowrate Specifications

---

Two commands can be used in the CRUde section to define the flowrate of a feed stream "j".

First, define the total flowrate of the feed stream "j" on a **dry** basis with the command below.

**FEEd dry** rate (Q units/t units) **j** =

Enter the flowrate for stream number "j". If you are specifying composition with a distillation curve or using a library crude oil, enter total feed flowrate (one value).

Second, define the flowrate of water in the feed stream "j" with the command below.

**FEEd WATER** (Q units/t units) **j** =

If water is present in a stream, enter its flow. This value is added to the FEEd rate value above.

---

## Crude Bulk Feed Temperature And Pressure Specifications

---

A temperature and pressure command is always required for each feed stream "j". Use the command below to specify these properties:

**TP** (T units, P units) **j** =

Enter the temperature and pressure of each feed "j", separated by a comma, where "j" is the stream number.

---

## Crude Bulk Feed Optional Properties

DESIGN II allows using the following specifications and options when the simulation contains a **CRUde** feed section.

---

## Crude Bulk Feed Molecular Weight Specifications

---

DESIGN II automatically assigns a molecular weight to each pseudocomponent, according to correlation techniques. The default correlation when using a **CRUde** or **REFine** section is Hariu. This correlation is reasonable for "light" crudes and most lean oils. However, the heavier or more aromatic the crude stream becomes, the less accurate the estimated molecular weight becomes. This can significantly affect prediction of K-values, enthalpies, and consequently feed vaporization. Four correlation options for estimating molecular weights are available. They are described in *Crude Bulk Feed Molecular Weight Estimation Options* Section.

You can, also, adjust molecular weights for a feed by entering a molecular weight curve for that feed. The commands for this are shown below.

**FEEd MOLEcular WEIght** **j** =

Enter molecular weights, separated by commas, corresponding to volume percents from your ASTM or TBP feed; "j" is the stream number.

**FEEd MOLEcular weight VOLume percents** **j** =

Enter volume percents, separated by commas, corresponding to the molecular weights on the FEEd MOLEcular WEIght command. This command is not required if the volume percents are the same as those entered on the FEEd VOLume percents command.

If a FEEd WEIght percents command was entered, the values entered here must be on a weight basis also.

**FEEd BULK MOLEcular weight** **j** =

Optionally, enter the bulk feed molecular weight for stream number "j" when you have also entered molecular weight versus volume percents. The molecular weight of each pseudocomponent will be adjusted to meet the specified bulk molecular weight. This command is not required, but it results in a more realistic curve.

---

## Crude Bulk Feed Property Specifications

---

A number of feed properties may be entered for crude streams in DESIGN II. These properties include viscosity, sulfur content, pour point, or any other data blendable on a weight, volume, or molar basis. Special blending methods are used for viscosity or pour point. Product properties are calculated from the feed properties and can be used as **REFine** module product specifications.

DESIGN II accepts property data as a function of volume or weight percent of feed distilled. It assigns the properties on a pseudocomponent-by-pseudocomponent basis, just as pseudocomponent boiling points were determined from the feed distillation curve. For this reason, bulk stream properties alone are not sufficient for DESIGN II to calculate pseudocomponent properties. Some indication of how the property changes with feed boiling point is required. Similarly, it is difficult for DESIGN II to extrapolate some properties (such as viscosity) from mid-distillation range data to the extreme ends of the distillation curve. Therefore, data points for zero and one hundred percent distilled points are always recommended.

### Viscosity

You can enter up to 15 sets of viscosity data for each feed. Each set is a viscosity versus percent distilled curve measured at a specified temperature. If there are multiple feeds, the same number of data sets must be entered for each feed. The viscosity data you enter is used to report a viscosity for each stream and for the **REFine** module product specification. It is not used for any equipment sizing calculations such as **LINE** pressure drop or **HEAt EXChanger** rating.

Viscosity data points and corresponding volume or weight percents are entered with the following commands. If your data does not include values for 0 and 100 volume percent, extrapolate your curves and enter values for the initial and end points.

**FEEd VIScosity SET h** (V units) **STR j** =

Enter up to 15 sets of viscosity data per feed, where "h" is the set number and "j" is the stream number and viscosities are given at each mid-volume percent. The same number of viscosity data sets must be entered for each feed.

**FEEd VIScosity VOLume percent SET h STR j** =

Enter the corresponding mid-volume percents for each set of viscosity data. If this command is not entered, the program

## Chapter 4

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uses the values entered on the FEEd VOLume command.

If a FEEd WEIght percents command was entered, the values entered here must be on a weight basis also.

The temperatures at which the sets of data were measured are entered with the following command.

**FEEd VIScosity TEMperature (T units) =**

Enter up to 15 temperatures, separated by commas, each corresponding to a set number. Temperatures for all sets are listed on one FEEd VIScosity TEMperature command, in order of set number. If no temperatures are specified, the program uses default values of 100F and 210 F for the first two sets.

In addition to the viscosity curves, you should also enter a bulk feed viscosity for each feed with the following command.

**FEEd BULk VIScosity SET h (V units) STR j =**

Enter the bulk feed viscosity at the temperature of set "h" for stream "j". The viscosity curve(s) will be adjusted to meet the bulk viscosities you enter. This command is used in conjunction with the FEEd VIScosity SET command.

### Other Property Specifications

Feed properties other than viscosity can also be entered as functions of volume or weight percents, including sulfur content, nitrogen content, and pour points. Any property you specify, except pour points, must be blendable on a weight, volume or molar basis. In addition, the same number of data sets must be entered for each feed if there are multiple feeds. You can enter a maximum of fifteen sets of data (curves). Pour point data is blended according to a special pour point method.

If you specify a property, DESIGN II will account for that property in calculating the products. For example, if you specify sulfur content, you will get an idea of sulfur distribution in products.

Property data points are entered using the following command. If your data does not include values for 0 and 100 volume percent, extrapolate your curves and enter values for the initial and end points.

**FEEd PROperty SET h (units) STR j = name, data points**

where,

**h** is the set number

**j** is the stream number

Name is an alphanumeric name up to 16 characters; e.g. SULFUR

Units are special codes as follows:

**VOL** blends property on volume basis

**WGT** blends property on weight basis

**MOL** blends property on molar basis

**PPT** is used for pour-point data Volume percents corresponding to the data points are entered with the following command

**FEEd PROperty VOLume percent SET h STR j =**

Enter the corresponding volume percents for property set "h" for stream "j".

If a FEEd WEIght percents command was entered, the values entered here must be on a weight basis also.

In addition to the property curves, you may enter the same property on a bulk basis for each stream using the following command:

**FEEd BULk PROperty SET h STR j =**

Enter the bulk feed property of data set "h" for stream "j". The property curve(s) will be adjusted to meet the bulk property entered.

A separate command is required for each property set for each feed stream, and the units option must be consistent with the FEEd PROperty SET command. DESIGN II will adjust the property curves to meet the bulk value, resulting in more realistic curves.

---

## Crude Bulk Feed Assigning a Name

---

**FEEd NAME j =**

Enter a name for stream "j". The name may have up to 16 characters.

---

## Crude Bulk Feed Back Blending Products to Recreate a Feed

---

In many cases, TBP or ASTM curves are available for products from an existing unit, but are not available for the feed. In such cases, you can enter the product curves as separate feeds which will be blended to recreate the feed. You can use either the MIX or VALve modules. However, data from an operating unit often contains inconsistencies because of poor light-ends analysis, mismatches in gaps, or overlap of adjacent products. Be sure you review the resultant feed generated by DESIGN II so that you can correct obvious errors or inaccuracies. If you wish to apply specific crude bulk feed blend, please review details at [Crude Bulk Feed Blending](#) section.

Optionally, users can also make use of the following command to control the characterization (gravity, average boiling cut points, molecular weight, etc...) of all the different crude oil feed curves used within a simulation. This allows given properties to be maintained for each defined crude oil cut curve distribution without the back-blending discussed above.

**FEEd BLEND x = y**



Enter this command to obtain uniform cut curve properties for each defined crude oil curve distribution. Here 'x' is the stream number and 'y' is the blend number. Program allows for up to 200 partially blended feeds and 200 streams per crude blend.

**Notes:**

1. FEEd BLEnd must be the first command for each feed crude curve stream.
2. Every feed to be blended with stream x would have the same blend number y (default is 1 and blend number ranges from 1 through 200).
3. If the blend command is used, it must be given for every crude feed stream defined on the flowsheet.
4. If streams are not blended with other streams, the command would still be given with the next available blend number. The blend numbers are in sequence beginning with 1 but later feeds blended with an earlier feed would repeat that number. For example, if the first stream uses blend 1 as in FEEd BLEND x1 = 1 and any later stream to be blended with it would also be FEEd BLEND x2 = 1. Here x1 & x2 are two stream numbers with same defined crude curve distribution. Other identical feed crude curve streams can be using same or different blend numbers, depending on user requirements on assay results.

---

## Crude Bulk Feed Critical Pressure Estimation Options

---

**DATa PC KEy =**

Enter option for prediction of critical pressure for petroleum fractions. Default option is CAVett. (choose one of the following options)

**CAVett**

This is the default correlation for calculating critical pressures for petroleum fractions. Reference 44.

**COAL liquids**

Correlation developed by Wilson, et.al. for calculating critical pressures for petroleum fractions, especially those with Watson characterization factors which are less than 11. References 43.

**HERZog**

Method for estimating critical pressure using vapor pressure, boiling points and parachors for substances. Works best for saturated and unsaturated hydrocarbons; accuracy decreases for aromatic and cyclic compounds. Reference 46.

**LEE**

Lee-Kesler technique is used to calculate critical pressures for petroleum fractions. References 25 and 31.

**WATson**

The Lee-Kesler correlation is used to calculate critical pressures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31 and 43.

---

## Crude Bulk Feed Critical Temperature Estimation Options

---

**DATa TC KEy =**

Enter option for prediction of critical temperature for petroleum fractions. Default option is CAVett. (choose one of the following options)

**CAVett**

This is the default correlation for calculating critical temperatures for petroleum fractions. Reference 44.

**COAL liquids**

Correlation developed by Wilson, et.al for estimating critical temperatures for petroleum fractions, especially those with Watson characterization factors which are less than 11. Reference 43.

**LEE**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions. References 25 and 31.

**NOKay**

Method for calculating critical pressure for paraffinic, olefinic, naphthenic and aromatic hydrocarbons with boiling points in the range of -40 to 1000F and specific gravities in the range of 0.5 to 1.0. Reference 45.

**WATson**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31, and 43.

---

## Crude Bulk Feed Molecular Weight Estimation Options

---

**DATa MOL KEy =**

Enter option for prediction of molecular weight for petroleum fractions. Default option for petroleum fractions entered in GENeral section is CAVett. Default option for CRUde feed description is HARiu. (choose one of the following options)

**CAVett**

This is the default option for predicting molecular weight when petroleum fraction commands are entered in the GENeral section (AMB i =, API i =). Reference 44.

**API**

Technique developed by M. Riazi at the Pennsylvania State University for calculating molecular weights of petroleum fractions. This technique should be avoided for light hydrocarbons (hexanes and lighter). Reference 48.

## Chapter 4

---

### HARiu

This is the default option for predicting molecular weights for petroleum fractions if you use any of the following in your simulation: REFine module, CRUDe feed section or PETroleum STReam print option. Reference 47.

### LEE

Lee-Kesler correlation for calculating molecular weights for petroleum fractions. Reference 25 and 31.

---

## Crude Bulk Feed Acentric Factor Estimation Options

---

At any time, additional thermophysical data for a particular component may be provided directly to DESIGN II for simulation calculation. The provided data will be used rather than allowing DESIGN II to estimate properties for the components specified. The acentric factors (ACE) may be entered in the GENERAL section of DESIGN II input. DESIGN II will use this data in subsequent calculations. The commands for entering this information are:

### ACE i =

Enter acentric factor for component "i". Default method is Edmister.

For additional command options please see *ChemTran: Acentric Factor*

---

## Crude Bulk Feed Step by Step

---

### Crude Bulk Feed STEP 1

---

#### Identify CRUDe input section ALWAYS REQUIRED.

Identify the crude feed definition section

CRU

---

### Crude Bulk Feed STEP 2

---

#### Enter light end analysis, if available.

If light-end analysis available for one or more feeds THEN assign each light-end (real) component and ID number from the database

list these ID numbers in the COM command of the GENERAL section following these stipulations **COM = 62, ..**

- water must always be the first component listed (ID = 62)
- list the remaining components in order of ascending boiling points

**NOTE:** Place the COM command only in the GENERAL section. The remaining instructions must appear in the CRUDe section of the input file.

Enter the individual (not cumulative) volume or weight percent for real components in exact order **FEE REA j =** as in COM command in GENERAL section. Entries are assumed to be volume % if FEE VOL command is also entered and weight % if FEE WEI command is entered.

**DO NOT ENTER A VALUE FOR WATER**

---

### Crude Bulk Feed STEP 3

---

#### Enter distillation curve cumulative volume or weight percent data.

Specify composition via distillation curve for each feed. Cumulative percent distilled (dry basis) for temperature

- volume percent
- weight percent

**FEE VOL j =**  
**FEE WEI j =**

---

### Crude Bulk Feed STEP 4

---

#### Enter distillation curve temperatures according to type of data available.

Temperatures at specified cumulative percentages (choose ONE of the following).

- True Boiling Point
- ASTM D-86
- ASTM D-1160 (760 mm)
- ASTM D-1160 (10 mm)

**FEE TBP (T units) j =**  
**FEE AST (T units) j =**  
**FEE AST HIGH (T units) j =**  
**FEE AST LOW (T units) j =**

---

### Crude Bulk Feed STEP 5

---

#### Enter feed gravity information based on the data available ALWAYS REQUIRED.

Gravity data for each feed (1 of 3 ways).

- Bulk feed gravity only
  - Average gravity of feed
- Gravity versus volume percent curve
  - cumulative volume percents
  - gravities at volume percents
  - optionally, enter feed bulk gravity

**FEE GRA (G units) j =**  
**FEE GRA VOL (G units) j =**  
**FEE GRA (G units) j =**  
**FEE BUL GRA (G units) j =**

---

- UOP characterization factor only
  - UOP factor for feed

FEE UOP j =

## Crude Bulk Feed STEP 6

**Supply flow data ALWAYS REQUIRED.** Feed flowrate data.

- Total dry feed flowrate
- Flowrate of water

FEE (Q units/t units) j =

FEE WAT (Q units/t units) j =

## Crude Bulk Feed STEP 7

**Supply temperature and pressure data ALWAYS REQUIRED.** Temperature and pressure of feed.

Temperature and pressure

TP (T units, P units)

## Crude Bulk Feed STEP 8

**Enter optional data.** Optional commands.

- Adjust pseudocomponent analysis
  - DESIGN II automatically generates pseudocomponents from the distillation curve specified. You can adjust the pseudocomponent slate in one of two ways.

Enter mean average boiling points for all pseudocomponents in ascending order. The complete feed must be covered from initial boiling point to end point. Only one CUT command is allowed per simulation

CUT (T units) =

- If no CUT command is used, these commands change the default temperature breaks of 600 and 800 F and adjust the default cut sizes, respectively. See *Crude Bulk Feed Composition Specifications*.

TEM BRE (T units) =

TEM INC (T units) =

- Molecular weight versus volume percent curve
  - Cumulative volume percents
  - Mole weights at volume percents
  - Optionally, enter feed bulk mole weight
- Feed viscosity data and other property specifications

FEE MOL VOL j =

FEE MOL WEI j =

FEE BUL MOL j =

- Viscosity and other feed properties can be entered as functions of volume percents. Any property specified, except for pour points, must be blendable on a weight, volume or molar basis. See *Crude Bulk Feed Property Specifications*.

Feed name, used in CRUde section output (up to 16 characters, no commas)

FEE NAM j =

## Crude Bulk Feed Example: Specification Using TBP Distillation Curve

Given the information below, specify the feed description for DESIGN II input.

### ENTER THE COMPOSITION

Define the Light Ends composition in the GENERAL section:

- **GENERAL**, **COMP**onents = 62, 2, 3, 4
- Initialize the CRUDE feed section
- **CRU**de

Enter the light end real component volume percents:

**FEEd REAL 1** = 0.12, 2.0, 1.9

### ENTER TEMPERATURE AND PRESSURE DATA

- **TP 1** = 625, 19.6

### ENTER FEED VISCOSITY DATA

- **FEEd VIS**cosity **TEM**perature = 100, 210
- **FEEd VIS**cosity **SET 1** (CST) **STR 1** = 0, 3.8, 6, 16, 52, 216, 1000, 2600, 39000
- **FEEd VIS**cosity **SET 2** (CST) **STR 1** = 0, 1.4, 1.8, 3.2, 5.9, 14, 30, 50, 245
- **FEEd VIS**cosity **VOL**ume **SET 1** **STR 1** = 0, 32, 38, 50, 60, 70, 75, 78, 100
- **FEEd VIS**cosity **VOL**ume **SET 2** **STR 1** = 0, 32, 38, 50, 60, 70, 75, 78, 100
- **FEEd BUL**k **VIS**cosity **SET 1** (CST) **STR 1** = 86
- **FEEd BUL**k **VIS**cosity **SET 2** (CST) **STR 1** = 7.8

### ENTER THE DISTILLATION CURVE

## Chapter 4

---

- FEEd TBP 1 = 50, 100, 175, 200, 400, 500, 700, 800, 900, 1000, 1100, 1300
- FEEd VOLume 1 = 0, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100

### ENTER FEED GRAVITY DATA

Enter bulk feed gravity data

- FEEd GRAvity (API) 1 = 22.5

### ENTER THE FEED FLOWRATE

- Enter total feed flow on a dry basis
- FEEd rate (BBL/DAY) 1 = 47400

### ENTER FEED SULFUR DATA:

- FEEd PROperty SET 1 (WGT) STR 1=SULFUR WT,0,.002,.002,.004,.032,.16,.46,.81,.94,1.11,1.57,2.38
- FEEd PROperty VOLume SET 1 STR 1 = 0, 5, 6.5, 10, 21, 30, 40, 50, 61, 71, 81.7, 100
- FEEd BULK PROperty SET 1 STR 1 = 0.94

### ENTER FEED NAME

- FEEd NAME 1 = SAMPLE CRUDE

Putting it all together, the complete feed specification section looks as follows. The feed specification commands are now ready to be added to an input file for a rigorous column or other DESIGN II equipment module simulation.

```
GENeral,
COMponents = 62, 2, 3, 4,
CRUde,
  FEEd TBP 1 = 50, 100, 175, 200, 400, 500, 700, 800, 900, 1000, 1100, 1300,
  FEEd VOLume 1 = 0, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100,
  FEEd GRAvity (API) 1 = 22.5,
  FEEd rate (BBL/DAY) 1 = 47400,
  FEEd REAL 1 = 0.12, 2.0, 1.9,
  TP 1 = 625, 19.6,
  FEEd VIScosity TEMperature = 100, 210,
  FEEd VIScosity SET 1 (CST) STR 1 = 0, 3.8, 6, 16, 52, 216, 1000 ,2600, 39000,
  FEEd VIScosity SET 2 (CST) STR 1 = 0, 1.4, 1.8, 3.2, 5.9, 14, 30, 50, 245,
  FEEd VIScosity VOLume SET 1 STR 1 = 0, 32, 38, 50, 60, 70, 75, 78, 100,
  FEEd VIScosity VOLume SET 2 STR 1 = 0, 32, 38, 50, 60, 70, 75, 78, 100,
  FEEd BULK VIScosity SET 1 (CST) STR 1 = 86,
  FEEd BULK VIScosity SET 2 (CST) STR 1 = 7.8,
  FEEd PROperty SET 1 (WGT) STR 1 = SULFUR WT, 0,.002, .002, .004, .032, .16, .46, .81, .94,1.11, 1.57,
  FEEd PROperty VOLume SET 1 STR 1 = 0, 5, 6.5, 10, 21, 30, 40, 50, 61, 71, 81.7, 100
  FEEd BULK PROperty SET 1 STR 1 = 0.94,
  FEEd NAME 1 = SAMPLE CRUDE
```

---

## Crude Bulk Feed Command Summary

---

### Input Section Identification

CRUde

### Composition Specifications

GENeral section entry:

COMponents = 62, ..

CRUde section entries:

FEEd REAL j =

FEEd ASTm (T units) j =

FEEd ASTm HIGH (T units) j =

FEEd ASTm LOW (T units) j =

FEEd TBP (T units) j =

FEEd VOLume percents j =

FEEd WEIght percents j =

CUT points (T units) =

TEMperature of BREaks (T units) =

TEMperature of INCRements (T units) =

### Feed Gravity Specifications

FEEd GRAvity (G units) j =

FEEd GRAvity VOLume percents j =

FEEd BULK GRAvity (G units) j =

### Flowrate Specifications

FEEd rate (Q units/t units) j =

FEEd WATer (q units/t units) j =

### Temperature and Pressure Specifications

TP (T units, P units) j =

### Molecular Weight Specifications

FEEd MOLEcular WEIght j =

FEEd MOLEcular weight VOLume percents j =

FEEd BULK MOLEcular weight j =

### Feed Viscosity Specifications

FEEd VIScosity SET h (V units) j =

FEEd VIScosity VOLume percent SET h j =

FEEd VIScosity TEMperature (T units) =

FEEd BULK VIScosity SET h (V units) j =

### Other Property Specifications

FEEd PROperty SET h (blending method) j =

FEEd PROperty VOLume percent SET h j =

FEEd BULK PROperty SET h j =

### Assigning a Feed Name

FEEd NAME j =

# Chapter 5: Component by Component Crude Streams

If you have a compositional breakdown of a feed from a previous simulation, you can specify it on a component-by-component basis instead of entering a distillation curve. This method is useful, for example, when you want to take the bottom product from an atmospheric tower simulation and enter it as a feed for a separate vacuum tower simulation. This section describes the commands used for component-by-component feed specification.

For each feed described in the CRUde section, the minimum required information is:

1. Composition
2. Gravity (API or Specific Gravity)
3. Flowrate
4. Temperature and Pressure

Each stream in your simulation must be numbered uniquely, including feed streams. All required specifications must be entered for each feed.

## Component by Component Command Details

### Component by Component Input Section Identification

The CRUde section of a DESIGN II input file must be distinct from other input sections; e.g., Title, Equipment Modules, etc. Therefore, initialize this section with the following command:

#### CRUde

Must be the first command in the CRUde section.

### Component by Component Crude Feed Composition Specifications

Component distillation data can be divided into two major portions; light-ends (real components) and pseudocomponents. Since light ends consist of identifiable chemical compounds (ethane, butanes, etc.), and since the properties for these compounds are contained in the *Database Components*, they are called real components. The remaining components are pseudocomponents, representing specific cuts of the crude feed.

Each real component and each pseudocomponent must have its own boiling point, flowrate, average gravity, and molecular weight. The following paragraphs explain how each portion is handled.

#### Light Ends Analysis

The following command is used to specify the light end analysis (real components) when component-by-component feed data is available.

The COMponents command must appear in the GENeral section of the input file.

#### COMponents =

- Enter component ID numbers separated by commas (from the *Database Components*) for all real components.
- A single COMponents command is used to list real components for **ALL** feeds in an input, regardless of the number of feeds.
- Water (ID=62) **must** be the first component listed in the COM= command.
- List remaining real components in order of ascending boiling point. Properties contained in the PURE COMPONENT DATABASE are automatically used for calculations.

You should also specify IMM=62 in the GENeral section, if you are not using a K-value option which automatically treats water as immiscible.

#### Pseudocomponents

Pseudocomponents are identified, on a component-by-component basis, by their mean average boiling points. Use the command below for this purpose.

#### CUT (T units) =

Enter the average boiling point for each pseudocomponent, in ascending order. There is only one CUT command allowed per run.

### Component by Component Feed Gravity Specification

A feed gravity specification is also required to characterize the pseudocomponents. Enter average gravities for the pseudocomponents with the FEEd COMponent GRAvity command. If you are combining feeds from multiple runs which have different gravities for the same cuts, use the FEE COM GRA j, and FEE COM GRA i commands, where "j" and "i" represent two stream numbers. DESIGN II blends these quantities on a volume basis.

#### FEEd COMponent GRAvity (G units) j =

Enter the average gravity for each pseudocomponent, in the same order as on the CUT command. If a stream number "j"

## Chapter 5

---

is entered as shown, the command will apply only to that stream. If no stream number is entered, the command will apply to all the CRUde section streams.

or

**FEEd COMpoment GRAvity** (G units) =

Enter the average gravity for all the pseudocomponents. This command will apply to all CRUde section streams.

Although only one CUT command is allowed per input, multiple FEE COM GRA = commands are permissible. If more than one FEE COM GRA = command is used, each should be assigned the appropriate stream number before the equals sign.

---

### Component by Component Flowrate Specifications

---

The flowrate of each component in each feed stream must be specified. Individual flowrates may be entered, or individual volume percents and a total flowrate may be entered. To enter flowrates for each component, specify values. Values are entered for all real components, including water, and all pseudocomponents.

**FEEd** (Q units/t units) j =

- Enter the flowrate for each real component in the same order as on the COMponents list (i.e. water first). Separate the component flowrates with commas.
- Continuing with the same FEE command, enter flowrates for each pseudocomponent in the same order as on the CUT command, separated by commas.
- Enter zeroes for components not present in stream number "j".

To enter component flowrates using volume percents and a total flowrate, enter the following commands.

**FEEd REAL** j =

Enter the individual volume percents for each real component excluding water, in the same order as they appear in the COMponents command in the GENeral section for stream "j". Separate entries with commas.

**FEEd PSEudocomponents** j =

Enter the individual volume percents for each pseudocomponent in stream "j", in the same order as they appear in the CUT command. Separate entries with commas.

**FEEd** (Q units/t units) j =

Enter the total flowrate for stream "j".

This option requires a CUT command and either FEE COM GRA or FEE COM GRj where j is the same stream number for which the volume percent data is entered.

---

### Component by Component Crude Temperature and Pressure Specifications

---

A temperature and pressure specification is always required in a DESIGN II input file.

**TP** (T units, P units) j =

Enter the temperature and pressure for each feed stream, where "j" is the feed stream number from your flowsheet.

## Component by Component Optional Commands

---

### Component by Component Molecular Weight Specification

---

The FEEd COMpoment MOLEcular weight command is optional, since DESIGN II automatically assigns molecular weights to each pseudocomponent from the CUT and FEE COM GRA information using correlation techniques. The default correlation when using a CRUde section is Hariu. This correlation is reasonable for "light" crudes and most lean oils. However, the heavier or more aromatic the crude stream becomes, the less accurate the estimated molecular weight becomes. This can significantly affect prediction of K-values, enthalpies, and consequently feed vaporization. Four correlation options for estimating molecular weights are available. They are described in *Molecular Weight Estimation Options*.

You may enter molecular weight data for each pseudocomponent with the following command.

**FEEd COMpoment MOLEcular weight** j =

Enter the molecular weights for each pseudocomponent in the same order as on the CUT command. If a stream number "j" is entered as shown, the command will apply only to that stream. If no stream number is entered, the command will apply to all the CRUde section streams.

---

### Component by Component Feed Viscosity Specifications

---

You can enter up to 15 sets of viscosity data for each feed. The viscosity sets are viscosity versus volume percent curve, measured at a specified temperature. If there are multiple feeds, the same number of data sets must be entered for each feed. The viscosity data you enter is used to report a viscosity for each stream and for the REFIne module product specifications. It is NOT used for any equipment sizing calculations such as LINE pressure drop or HEAT EXChanger rating.

Viscosity sets are entered with the following commands:

## Component by Component Crude Streams

---

### **FEEd COM**ponent **VIS SET h** (V units) **STR**eam **j** =

Enter values for viscosities for each pseudocomponent in stream j.

where h is the set number (maximum of 15)

V units are the dimensional units for viscosities (default is centistokes (CST))

j is the stream number

### **FEEd VIS**cosity **TEM**peratures (T units) =

Enter the temperatures at which each set of viscosity data was measured, beginning with SET 1. If this command is not entered, default values of 100 and 210o F will be used.

In addition to the viscosity data, you should also enter a bulk feed viscosity for each feed with the following command.

### **FEEd BULk COM**ponent **VIS**cosity **SET h** (V units) **STR j** =

Enter the bulk component by component feed viscosity at the temperature of set "h" for

stream "j". The viscosity curve(s) will be adjusted to meet the bulk viscosities you enter.

This command is used in conjunction with the FEEd COMponent VIScosity SET h STR j command.

---

## Component by Component Other Property Specifications

---

Feed properties other than viscosity, such as sulfur content, nitrogen content, and pour points, can also be entered as functions of volume percent. Any property you specify, except pour points, must be blendable on a weight, volume or molar basis. In addition, the same number of data sets must be entered for each feed if there are multiple feeds. You can enter a maximum of fifteen sets of data (curves).

If you specify a property, DESIGN II will account for that property in calculating the products. For example, if you specify sulfur content, you will get an idea of sulfur distribution in products.

Property data points are entered using the following command. If your data does not include values for 0 and 100 volume percent, extrapolate your curves and enter values for the initial and end points.

### **FEEd COM**ponent **PRO**perty **SET h** (units) **STR j** = name, data points

where,

**h** is the set number

**j** is the feed number

Units are special codes as follows:

**VOL** blends property on volume basis

**WGT** blends property on weight basis

**MOL** blends property on molar basis

**PPT** used for pour-point data

name = 16 character user-assigned property name, e.g.: SULFUR. Each feed must use the same name for a given set. NO commas are allowed in the name.

**NOTE:** Both the viscosity and property set data require the CUTS, FEEd COMponent GRAvity and FEEd PSEudocomponent commands.

### **FEEd NAME j** =

Enter the name for stream j, up to a maximum of 16 characters. No commas are allowed in the name.

---

## How to Enter Component-by-Component Properties

---

The guidelines below outline what commands are required and what commands are optional when defining a stream with component-by-component properties which include pseudocomponents..

The following commands are required:

**CRU**de

**CUT**=

mean average boiling points for all pseudocomponents)

**FEEd COM**ponent **GRA**vity **j** =

(or **FEEd COM**ponent **GRA**vity = )

**TP j** =

**FEEd** rate **j** =

The following commands are required to define viscosity:

**FEEd PSE**udocomponents **j** =

(Volume % for each pseudocomponent in stream j) This is optional for feed description but required for viscosity property sets

**FEEd COM**ponent **VIS**cosity **SET h STR**eam **j** =

## Chapter 5

**FEEd VIScosity TEMperatures** (T units) =

The following command is required to define other properties:

**FEEd COMponent PROperty SET h** (units) **STReam j** =

The following commands are optional:

**FEEd COMponent MOLe weight j** =

(or **FEEd COMponent MOLe weight =** ) **FEEd NAME j** =

**NOTE:** For clarity, keywords are shown with their complete spellings using capitals and lowercase letters.

Only those letters shown in CAPitals are actually required by DESIGN II.

### Restrictions on Component-by-Component Property Commands

The following restrictions apply:

1. Each feed must have the same number of property and viscosity sets.
2. It is permissible to use FEEd COMponent PROperty SET and FEEd PROperty SET in the same run, as long as only one is entered for a given feed. The same applies to FEEd COMponent VIScosity SET and FEEd VIScosity SET.
3. For any given property set, the same mixing rule option and property name must be used for all feeds.
4. The VIScosity TEMperature command applies to all viscosity sets and should have one value entered for each viscosity set.

## Component by Component Assigning a Name

**FEEd NAME j** =

Enter a name for feed stream "j". The name may have up to 16 characters.

## Component by Component Crude Feed Command Summary

### Input Section Identification

**CRUde**

### Composition Specifications

**GENeral section entry:**

**COMponents** = 62, ..

### Pseudocomponent Boiling Points

**CUT** (T units) =

### Pseudocomponent Gravity

**FEEd COMponent GRAvity** (G units) j =

or

**FEEd COMponent GRAvity** (G units) =

### Pseudocomponent Molecular Weight

**FEEd COMponent MOLeclar weight j** =

or

**FEEd COMponent MOLeclar weight** =

### Flowrate Specifications

**FEEd** (Q units/t units) j =

### T and P Specifications

**TP** (T units, P units) j =

### Feed Viscosity Specifications

**FEEd PSEudocomponents j** =

**FEEd COMponent VIScosity SET h** (V units) j =

**FEEd VIScosity SET h** (V units) j =

**FEEd VIScosity VOLume percent SET h** (V units) j =

**FEEd VIScosity TEMperature** (T units) =

**FEEd BULk COMponent VIScosity SET h** (V units) j =

### Other Property Specifications

**FEEd PROperty SET h** (blending method) j =

**FEEd PROperty VOLume percent SET h j** =

**FEEd BULk PROperty SET h j** =

### Assigning a Feed Name

**FEEd NAME j** =

## Component by Component Examples

Given the following component data, prepare a DESIGN II input file specifying the feed stream.

### Bulk Properties

Temperature: 625 F  
 Pressure: 29.7 PSIA  
 Flow rate: 15738E7 LB/HR  
 Feed Name: SAMPLE  
 Sulfur Content: 0.94 weight %

### Light End Analysis

Water 50 LB/HR  
 Methane .14 VOL %  
 Ethane .96  
 Propane 1.2  
 i-Butane 0.7  
 n-Butane 2.5  
 n-Pentane 3.5

### Viscosity

@ 100 F @ 210 F Pseudocomponent

### Centistokes

4.012	1.438	200 ABP
4.649	1.558	225 ABP
5.197	1.658	250 ABP
5.952	1.792	275 ABP
7.283	2.014	300 ABP
9.649	2.374	350 ABP
13.02	2.833	400 ABP
19.52	3.554	450 ABP
38.04	5.026	500 ABP
78.52	7.493	550 ABP
160.4	11.59	600 ABP



# Component by Component Crude Streams

## Sulfur Distribution

Weight % Sulfur	Pseudocomponent	303.9	16.82	650 ABP
.01167	200 ABP	527.3	22.24	700 ABP
.03851	225 ABP	902.3	28.64	750 ABP
.08584	250 ABP	1314.0	34.54	800 ABP
.1636	275 ABP	1732.0	39.95	850 ABP
.3032	300 ABP	2297.0	46.61	900 ABP
.5198	350 ABP	8430.0	127.3	1000 ABP
.7210	400 ABP	.6862E5	673.6	1100 ABP
.8740	450 ABP	.4273E6	2881.0	1200 ABP

Bulk viscosity: 25.0 5.0

## Pseudocomponent Data

	MABP, F	Vol %	API	MW
1.024	550 ABP			
1.112	600 ABP	200	10.46	62.6
1.212	650 ABP	225	3.955	53.8
1.355	700 ABP	250	4.113	49.0
1.523	750 ABP	275	4.126	45.6
1.683	800 ABP	300	6.214	42.3
1.806	850 ABP	350	5.915	40.1
1.958	900 ABP	400	5.187	36.4
2.132	1000 ABP	450	5.685	32.6
2.299	1100 ABP	500	5.705	29.0
2.446	1200 ABP	550	5.065	25.9
Bulk Feed Sulfur: 0.94 weight %	600	600	4.872	23.8
	650	650	3.618	22.0
	700	700	3.618	20.2
	750	750	3.268	18.4
	800	800	2.671	16.8
	850	850	2.671	15.4
	900	900	3.895	13.5
	1000	1000	3.558	10.8
	1100	1100	3.574	7.5
	1200	1200	2.647	5.1

## **ENTER THE COMPOSITION**

Define the Light Ends (or real components) composition in the GENeral section

**GENERAL, COM**ponents = 62, 2, 3, 4, 5, 6, 8

Initialize the CRUDE feed section

**CRU**de,

Define the pseudocomponents composition with the CUT= command

**CUT**(F)=200, 225, 250, 275, 300, 350, 400, 450,  
500, 550, 600, 650, 700, 750, 800, 850, 900, 1000, 1100, 1200

## **ENTER PSEUDOCOMPONENT GRAVITY DATA**

Enter gravity data for each pseudocomponent

**FEE COM GRA** (API)1=62.6,53.8,49.,45.6,42.3,  
40.1,36.4,32.6,29.,25.9,23.8,22.,20.2,18.4, 16.8,15.4,13.5,10.8,7.5,5.1

## **ENTER THE FEED FLOWRATE**

First, enter the total flowrate

**FEE** (LB/HR) 1 = 1573800.

Then enter the water rate

**FEE WAT**(LB/HR) 1 = 50.

Next enter the volume percents for the real components

**FEE REA** 1 = 0.14,0.96,1.2,0.7,2.5,3.5,

Finally, enter the volume percents for the pseudocomponents

**FEE PSE** 1 = 10.146,3.955,4.113,4.126,6.214,  
5.915,5.187,5.685,5.705,5.065,4.872,3.618,  
3.618,3.268,2.671,2.671,3.895,3.558,3.574, 2.647,

## **ENTER TEMPERATURE AND PRESSURE DATA**

Specify the feed temperature and pressure

**TP** (F,PSIA) 1 = 625, 29.7

## **ENTER PSEUDOCOMPONENT MOLECULAR WEIGHT DATA**

Enter optional molecular weight of each pseudocomponent

**FEE COM MOL** 1 = 99.36,103.,108.5,114.88,  
121.54,138.39,155.69,174.01,193.71,215.31,  
239.42,265.66,293.62,323.22,354.77,388.17,

## Chapter 5

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421.38,495.25,568.58,648.47,

### ENTER FEED VISCOSITY DATA

FEE VIScosity TEMperature (F) = 100, 210

FEE COM VIS SET 1 (CST) STR1=4.012, 4.649, 5.197, 5.952, 7.283, 9.649, 13.02, 19.52, 38.04, 78.52, 160.4, 303.9, 527.3, 902.5, 1314., 1732., 2297., 8430., 68620., 427300.,

FEE COM VIS SET 2 (CST) STR1=1.438, 1.558, 1.658, 1.792, 2.014, 2.374, 2.833, 3.554, 5.026, 7.493, 11.59, 16.82, 22.24, 28.64, 34.54, 39.95, 46.61, 127.3, 673.6, 2881.,

FEE BULK COM VIS SET 1 (CST) STR1=25.0

FEE BULK COM VIS SET 2 (CST) STR2=5.0

### ENTER FEED SULFUR DATA

FEE COM PROP SET 1 (WGT) STR 1=SULFUR WT,

.01167, .03851, .08584, .1636, .3032, .5198, .721, .874, .943, 1.024, 1.112, 1.355, 1.523, 1.683, 1.806, 1.958, 2.132, 2.299, 2.446,

### ENTER FEED NAME

FEE NAME 1 =SAMPLE

Putting it all together, the complete feed specification section looks as follows. The feed specification commands are now ready to be added to an input file for a rigorous column, or other DESIGN II equipment module simulation.

GENeral,

COMponents = 62, 2, 3, 4, 5, 6, 8

CRUde,

CUT(F)=200, 225, 250, 275, 300, 350, 400, 450,  
500, 550, 600, 650, 700, 750, 800, 850, 900, 1000, 1100, 1200

FEE COM GRA (API)1=62.6,53.8,49.,45.6,42.3,  
40.1,36.4,32.6,29.,25.9,23.8,22.,20.2,18.4, 16.8,15.4,13.5,10.8,7.5,5.1

FEE (LB/HR) 1 = 1573800.

FEE WAT(LB/HR) 1 = 50.

FEE REA 1 = 0.14,0.96,1.2,0.7,2.5,3.5,

FEE PSE 1 = 10.146,3.955,4.113,4.126,6.214,  
5.915,5.187,5.685,5.705,5.065,4.872,3.618,  
3.618,3.268,2.671,2.671,3.895,3.558,3.574, 2.647,

TP (F,PSIA) 1 = 625, 29.7

FEE COM MOL 1 = 99.36,103.,108.5,114.88,  
121.54,138.39,155.69,174.01,193.71,215.31,  
239.42,265.66,293.62,323.22,354.77,388.17,  
421.38,495.25,568.58,648.47,

FEE VIScosity TEMperature (F) = 100, 210

FEE COM VIS SET 1 (CST) STR1=4.012, 4.649,  
5.197, 5.952, 7.283, 9.649, 13.02, 19.52,  
38.04, 78.52, 160.4, 303.9, 527.3, 902.5,  
1314., 1732., 2297., 8430., 68620., 427300.,

FEE COM VIS SET 2 (CST) STR1=1.438, 1.558,  
1.658, 1.792, 2.014, 2.374, 2.833, 3.554,  
5.026, 7.493, 11.59, 16.82, 22.24, 28.64,  
34.54, 39.95, 46.61, 127.3, 673.6, 2881.,

FEE BULK COM VIS SET 1 (CST) STR1=25.0

FEE BULK COM VIS SET 2 (CST) STR2=5.0

FEE COM PROP SET 1 (WGT) STR 1=SULFUR WT,  
.01167, .03851, .08584, .1636, .3032,  
.5198, .721, .874, .943, 1.024, 1.112,  
1.355, 1.523, 1.683, 1.806, 1.958, 2.132, 2.299, 2.446,

FEE NAME 1 =SAMPLE

END

### ENTER THE COMPOSITION

Define the Light Ends (or real components) composition in the GENERAL section

GENERAL, COMponents = 62, 2, 3, 4, 5, 6, 8

Initialize the CRUDE feed section

CRUde,

Define the pseudocomponents composition with the CUT= command CUT(F)=200, 225, 250, 275, 300, 350, 400, 450,

# Component by Component Crude Streams

500, 550, 600, 650, 700, 750, 800, 850, 900, 1000, 1100, 1200

## ENTER PSEUDOCOMPONENT GRAVITY DATA

Enter gravity data for each pseudocomponent

**FEE COM GRA** (API)1=62.6,53.8,49.,45.6,42.3,40.1,36.4,32.6,29., 25.9,23.8,22.,20.2,18.4,16.8,15.4,13.5,10.8,7.5,5.1

## ENTER THE FEED FLOWRATE

First, enter the total flowrate

**FEE** (LB/HR) 1 = 1573800.

Then enter the water rate

**FEE WAT**(LB/HR) 1 = 50.

Next enter the volume percents for the real components

**FEE REA** 1 = 0.14,0.96,1.2,0.7,2.5,3.5,

Finally, enter the volume percents for the pseudocomponents

**FEE PSE** 1 = 10.146,3.955,4.113,4.126,6.214,5.915,5.187,5.685,  
5.705,5.065,4.872,3.618,3.618,3.268,2.671,2.671,3.895,3.558, 3.574,2.647,

## ENTER TEMPERATURE AND PRESSURE DATA

Specify the feed temperature and pressure

**TP** (F,PSIA) 1 = 625, 29.7

## ENTER PSEUDOCOMPONENT MOLECULAR WEIGHT DATA

Enter optional molecular weight of each pseudocomponent

**FEE COM MOL** 1 = 99.36,103.,108.5,114.88,121.54,138.39,155.69,  
174.01,193.71,215.31,239.42,265.66,293.62,323.22,354.77,388.17, 421.38,495.25,568.58,648.47,

## ENTER FEED VISCOSITY DATA

**FEE VIS**cosity **TEM**perature (F) = 100, 210

**FEE COM VIS SET 1** (CST) **STR**1=4.012,4.649,5.197,5.952,7.283,  
9.649,13.02,19.52,38.04,78.52,160.4,303.9,527.3,902.5,1314., 1732.,2297.,8430.,68620.,427300.,

**FEE COM VIS SET 2** (CST) **STR**1=1.438,1.558,1.658,1.792,2.014,  
2.374,2.833,3.554,5.026,7.493,11.59,16.82,22.24,28.64,34.54, 39.95,46.61,127.3,673.6,2881.,

**FEE BULK COM VIS SET 1** (CST) **STR**1=25.0

**FEE BULK COM VIS SET 2** (CST) **STR**2=5.0

## ENTER FEED SULFUR DATA

**FEE COM**ponent **PROP**erty **SET** 1 (WGT) **STR** 1=SULFUR WT.,01167.,03851,  
.08584.,1636.,3032.,5198.,721.,874.,943,1.024,1.112,1.355,1.523,1.683,1.806,1.958,2.132,2.299,2.446,

## ENTER FEED NAME

**FEED NAME** 1 =SAMPLE

Putting it all together, the complete feed specification section looks as follows. The feed specification commands are now ready to be added to an input file for a rigorous column, or other DESIGN II equipment module simulation.

```
GENeral,  
  COMponents = 62, 2, 3, 4, 5, 6, 8  
CRUDE,  
CUT(F)= 200, 225, 250, 275, 300, 350, 400, 450, 500, 550, 600,  
650, 700, 750, 800, 850, 900, 1000, 1100, 1200,  
FEE COM GRA(API) 1= 62.6,43.8,49.,45.6,42.3,40.1,36.4,32.6,29.,  
25.9,23.8,22.,20.2,18.4,16.8,15.4,13.5,10.8,7.5,5.1,  
FEE (LB/HR) 1 = 15373800.,  
FEE WAT (LB/HR) 1 = 50.,  
FEE REA 1 = 0.14,0.96,1.2,0.7,2.5,3.5,  
FEE PSE 1 = 10.646,3.955,4.113,4.126,6.214,5.915,5.187,5.685,  
5.705,5.068,4.872,3.618,3.618,3.268,2.671,2.671,3.895,3.558, 3.574,2.647,  
TP (F,PSIA)1=625, 29.7  
FEE COM MOL 1 = 99.36,103.,108.5,114.88,121.54,138.39,155.69,  
174.01,193.71,215.31,239.42,265.66,293.62,323.22,354.77,388.17, 421.38,495.25,568.58,648.47,  
FEE VIS TEM(F) = 100., 210.,  
FEE COM VIS SET 1 (CST) STR 1=4.012,4.649,5.197,5.952,7.283,9.649,  
13.02,19.52,38.04,78.52,160.4,303.9,527.3,902.5,1314.,1732.,2297., 8403.,68620.,427300.  
FEE COM VIS SET 2 (CST) STR 1=1.438,1.558,1.658,1.792,2.018,2.374,  
2.833,3.554,5.026,7.493,11.59,16.82,22.24,28.64,34.54,39.95,46.61, 127.3,673.6,2881.,  
FEE BULK VIS SET 1 (CST) STR 1 = 25.,  
FEE BULK VIS SET 2 (CST) STR 1 = 5.,  
FEE COM PROP SET 1 (WGT) STR 1=.01167.,.03851,.08584.,.1636.,.3032,  
.5198.,.721.,.874.,.943,1.024,1.112,1.212,1.355,1.523,1.683,1.806, 1.958,2.132,2.299,2.446,  
FEE NAM 1 = SAMPLE
```



# Chapter 6: Crude Oil Library

Properties of 38 of the crude feed stocks available from producing fields around the world are easily retrieved from the DESIGN II library using a simple keyword command for each crude oil. The only other feed information that you must provide is feed rate, temperature and pressure. You can combine more than one feed stock in a MIXer to get a desired blend. The names for the available crude oils are listed in the crude oil library table. You should enter the names exactly as they are listed. The crude oil data is taken from a series of articles published in the *Oil and Gas Journal* by Leo R. Aalund.

## Crude Oil Library Table

The crude feed names in the DESIGN II library are as follows:

ABU DHABI - MURBAN	NIGERIA - QUA IBOE
CEUTA - ZULIA	NORWAY - STATFJORD
INDONESIA - ATTAKA E. KALIMANTAN	QATAR - DUCKHAN
IRAN - ARDESHIR	QATAR - MARINE
IRAN - LIGHT (BASRAH)	SAUDI - BERRI
IRAN - DARIUS	SAUDI - HEAVY
IRAN - FEREIDOON BLEND	SAUDI - LIGHT
IRAN - HEAVY (BASRAH)	SAUDI - MEDIUM
IRAN - SASSAN	SAUDI - ZULUF
KUWAIT - KUWAIT CRUDE	U.K. - BUCHAN, NORTH SEA
LATIN - OFICINA	U.K. - FLOTTA MIX, NORTH SEA
LIBYA - AMNA (HIGH POUR)	U.K. - FORTIES
LIBYA - BREGA	U.K. - MAGNUS, NORTH SEA
MALAYSIA - TEMBUNGO	U.K. - NINIAN BLEND, NORTH SEA
NIGERIA - ESCRAVOS	U.K. - TARTAN, NORTH SEA
NIGERIA - FORCADOS BLEND	U.S. - N. DAKOTA (NORTHERN)
NIGERIA - LIGHT (BONNY)	U.S. - N. SLOPE
NIGERIA - MEDIUM (BONNY)	U.S. - ROCKY MOUNTAIN SWEET
NIGERIA - PENNINGTON	VENEZUELA - LAGOMEDIO

## Crude Oil Library Command Details

### Crude Oil Library Feed Stream Initialization

The commands for selecting a crude from the world library must appear in the CRUde section of the input file. The CRUde section of a DESIGN II input file must be distinct from other input sections; e.g., Title, Equipment Modules, etc. Therefore, initialize this section with the following command.

#### CRUde

Must be the first command in the CRUde section.

### Crude Oil Library Composition Specification

The following command is used to request one or more of the crude oils in the DESIGN II library.

#### FEEd STK j =

Enter the name of the feed stock for stream "j" from the library of world crudes.

### Crude Oil Library Flowrate Specification

Once the CRUDE LIBRARY selection(s) is made, you must specify the flowrate of the stream. Use the following command to specify the flowrate.

#### FEEd dry rate (Q units/t units) j =

Enter the flowrate for stream number ' j '. Enter total feed flowrate (one value).

Define the flowrate of water in the feed stream j with the command below.

#### FEEd WATer (Q units/t units) j =

If water is present in a stream, enter its flow. This value is added to the FEEd rate value above.

## Chapter 6

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### Crude Oil Library Temperature and Pressure Specification

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A selection from the CRUDE LIBRARY also requires the specification of the feed temperature and pressure. Use the following command to enter this required data.

**TP** (T units, P units) j =

Enter the temperature and pressure of each feed, where "j" is the stream number.

### Crude Oil Library Command Summary

**Input Section Identification**

**CRUde**

**Composition Specifications**

**FEEd STK j =**

**Flowrate Specification**

**FEEd rate (Q units/t units) j =**

**FEEd WATer (Q units/t units) j =**

**Temperature and Pressure Specification**

**TP (T units, P units) j =**

### Crude Oil Library Example

Specify a feed stream of 50000 bbl/day of ABU DHABI - MURBAN crude at 650 F and 27 PSIA.

**CRUde,**

**FEEd STK 1 = ABU DHABI - MURBAN**

**FEEd dry rate (BBL/DAY) 1 = 50000**

**TP 1 = 650,27**

# Chapter 7: Thermodynamics

DESIGN II has a comprehensive set of K-value, Enthalpy, Density, Transport (Viscosity and Thermal Conductivity) Properties, and Surface Tension of mixture correlations. These correlations can be used to model processes ranging from gas processing to refinery operations to petrochemicals and specialty chemicals. General recommendations as to the applicability of particular correlations are given below.

Any K-value, enthalpy or density commands entered in the GENeral section apply to all calculations within the simulation unless you enter K-value, enthalpy, or density commands for specific equipment modules.

## Thermodynamics: K-Value Options

### Thermodynamics: Water K-Values in Hydrocarbon Systems

(choose any of the following options)

#### IMMiscible =

Enter the component ID number for the component that is to be treated as immiscible. Water (component ID 62) is treated as a special case. If the IMMiscible calculation is specified for any component other than water, the calculation is based on three assumptions:

1. the vapor phase will be saturated with the immiscible component in a manner similar to the procedure described below for water.
2. for calculations with one or two outlet streams, the flowrate for the immiscible component will be reported separately from the portion of the immiscible component which is soluble in the hydrocarbon liquids.
3. for VALve or FLAsh calculations with three outlet streams, the two liquid phases will have a mutual solubility of 0.01 mol percent.

For the immiscible water calculation, DESIGN II first determines if sufficient water is present to form a third phase. If so, the vapor phase is saturated and water solubility in the hydrocarbon liquid phase is calculated. For calculations with one or two outlet streams, the flowrate for the immiscible water will be reported in the detailed stream summary separately from the water which is soluble in the hydrocarbon liquids. For FLAsh or VALve calculations with three outlet streams, the solubility of hydrocarbons in the "free water" phase is also calculated.

If sufficient water is present to form a third phase at the stream temperature, pressure, and composition, the water will be distributed between hydrocarbon vapor and liquid phases in accordance with the following equation:  $K_{\text{water}} = Y_{\text{water}}/X_{\text{water}}$ , where  $Y_{\text{water}}$  is the saturated vapor mole fraction and  $X_{\text{water}}$  is the solubility of water in liquid hydrocarbons at the stream temperature.

**NOTE:** Only one component can be declared immiscible per simulation.

#### STEam TABLES

The NBS/NRC steam tables are available for use in your process simulation. These equations will provide improved values for water enthalpies, densities, and transport properties such as viscosity, thermal conductivity, and surface tension. Steam tables will be used for any pure water stream (+99.99%), irrespective of the chosen thermodynamic method(s).

#### GPA WATER

Enter this command in the GENeral section, to have the vapor phase saturation predicted by the IMMiscible calculation for water in accordance with the chart in the *Engineering Data Book* (Gas Processors Suppliers Association, Chapter 15, page 15-10, 1976; original chart published in *Hydrocarbon Processing*, Vol. 37, No. 8, page 153 (1958) in an article by J.J. McKetta and A.H. Wehe). This chart has an upper temperature limit of 300F but the program will extrapolate.

#### SOLubility of WATER = COMPONENT

Enter this command to calculate water solubility in liquid hydrocarbons on a component basis rather than using the default water-in-kerosene calculation. DESIGN II has two methods for calculating water solubility in hydrocarbons. The default correlation uses the water-in-kerosene line (*Technical Data Book*, Figure 9A1.4, page 9-15, American Petroleum Institute, 1970) and is reasonable for most hydrocarbon-water systems. For light hydrocarbons, such as propane with water, the second correlation (*Technical Data Book*, Figure 9A1.5-1, page 9-17, American Petroleum Institute, 1970) shows significant improvement in solubility prediction. To use the second water solubility correlation, enter the SOL WAT = COM command in the GENeral section.

#### NO IMMiscible

Enter this command in the GENeral (or appropriate equipment modules) section to have water treated miscibly when using K-value options that normally assume water-hydrocarbon mixtures are immiscible.

#### USE LIQUID CP

This method is specifically used for only liquid mixtures. This command causes DESIGN II to evaluate each liquid stream automatically irrespective of the thermodynamic method(s) used for all systems. It will use mole fraction mixing rules for calculating the enthalpy of the mixture from the individual component enthalpies. An excess enthalpy correction is made

## Chapter 7

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for Glycol-Water (ID#62) systems, where glycols can be one among Ethylene Glycol (ID# 3103); Di-Ethylene Glycol (ID# 4030); Tri-Ethylene Glycol (ID# 4044); Propylene Glycol (ID#4031). The equations used will provide improved values for water-glycol enthalpies, densities, and transport properties such as viscosity, thermal conductivity, and surface tension. A liquid heat transfer fluid, THERMINOL 55-ID#2055 & THERMINOL 66-ID#2054 (copyrights Solutia Inc.) can also use this method for heat exchanger calculations.

**NOTE:** USE LIQ CP over-rides both stream and equipment specific thermodynamic options, if specified.

### Method of Calculation

This method is an approximation of the thermodynamics describing the equilibrium between a vapor, a liquid hydrocarbon, and a liquid water phase. This model assumes that

1. there are no hydrocarbons dissolved in the liquid water phase and
2. the amount of water in the liquid phase is determined by the water-in-kerosene correlation or the SOL WAT = COM technique.

These are reasonable approximations since the mutual solubilities of the hydrocarbons and water are very small. Given the amount of water in the vapor phase, the model then uses either the K-value option (GENERAL section or equipment specific) or the GPA WATER technique for modeling the distribution of water between the vapor phase and the hydrocarbon liquid. The amount of water kept in the vapor phase is the amount that would saturate the vapor phase in equilibrium with the pure water phase. Water in excess of the amount required for saturation going into the vapor phase from the liquid hydrocarbon phase is placed in the liquid water phase.

The default option for the solubility of water in hydrocarbons uses Figure 9A1.4, page 9-15 of the API Technical Data Book (water in kerosene, 1970 edition). The second option for water solubility in hydrocarbon liquids is on a component basis. This option is specified by entering a SOLubility of WATER = COMponent basis command in the GENERAL section. Solubilities in this section are dependent on the carbon to hydrogen weight ratio. The default carbon to hydrogen ratio for petroleum fractions can be overridden with the GENERAL section command, CARbon to HYDrogen weight ratio  $j =$  , where "j" is the component ID number. The reference for the water solubility on a component basis is Equation 9A1.5-1, page 9-17 of the API Technical Data Book (1970 edition). The hydrocarbon solubility in the "free water" phase is calculated using the technique described in Calculator Programs for the Hydrocarbon Processing Industries, (Vol. 2, page 41, Gulf Publishing Co., 1982).

An estimate of the amounts of H<sub>2</sub>S, CO, CO<sub>2</sub>, and NH<sub>3</sub> in the "free water" phase is made automatically using the APISOUR correlation.

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## Thermodynamics: K-Value Commands

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The list of K-value options will be divided into four groups according to their applicability to basic industry groups. The first group of K-value options is generally recommended for the natural gas processing and petroleum refining industries. The second group contains K-value options recommended for the petrochemical and chemical industries. The third and fourth sets of K-value options consist of tabular data and specialized options.

### Gas Processing and Petroleum Refining Recommended K-value Options

Water is assumed to be essentially immiscible (non-soluble) with hydrocarbons for the following K-value options: STDK, APISOAVEK, BRAUN, BWRK, BWRSK, CHAO, ESSO, ESSO TAB, KVAL, LKPK, MOD ESSO, RKK and SOAVEK. Water is assumed to be immiscible in the PENK option. If you want water to be treated as a miscible component when using the PENK option you should enter **NO IMM** in the GENERAL section or use MOD PENK which treats water as miscible species by default.

The name on the left is the appropriate keyword spelling for the K-value options. A description of the technique is given on the right. The default K-value option is PENK.

#### STDK

This method uses a combination of regular solution theory for activity coefficients and empirical functions to describe the liquid phase with the Redlich-Kwong equation for the vapor phase. The correlation was developed for hydrocarbons, hydrogen and gas oils and should give reasonable values for temperatures from 60 F to 800 F (or below critical temperature of mixture) for pressures up to 3000 PSIA. It should be used with caution at pressures above 600 PSIA or at temperatures below atmospheric. It is unreliable for systems containing more than a few mole percent of hydrogen sulfide or carbon dioxide. It should also not be used for modeling separations of close-boiling components (e.g. xylenes separation). Water is assumed to be immiscible for this option. References 2 and 4.

#### APISOAVEK

The American Petroleum Institute has generated interaction parameters for H<sub>2</sub>S, CO<sub>2</sub>, CO and N<sub>2</sub> with several hydrocarbons to be used with the SOAVE equation of state. This technique also contains a special equation for modeling hydrogen in hydrocarbon mixtures. For components not in *Thermodynamics Table 1. APISOAVEK Interaction Parameter List*, DESIGN II will use a component's solubility parameter to estimate binary interaction parameters for the SOAVE equation or you can regress your own VLE data via ChemTran. Water is assumed to be immiscible for this option. This K-value option may be used to regress equilibrium data (CHEMtran FILE required). If no data is fitted, K-values are generated from the equation of state. References 3 and 4.

#### BRAUN

The Braun K-10 technique is reasonable for aliphatic feeds at pressures below 100 PSIA. As feeds become increasingly aromatic or naphthenic, the accuracy decreases. Water is assumed to be immiscible for this option. Reference 6.



## BWRK

This is an application of the Benedict-Webb-Rubin equation of state. It is an eleven parameter equation developed for light hydrocarbon mixtures containing methane through pentane, nitrogen and carbon dioxide in the range of 26 F to 400 F. Water is assumed to be immiscible for this option. Computational time required for this option is much greater than that for the cubic equations of state. References 7a-d.

## BWRSK

This is an application of the 11 parameter Benedict-Webb-Rubin equation of state by Starling, et. al. It has an extended list of interaction coefficients and generalized correlation for parameters by Starling. It is very accurate for hydrocarbon mixtures containing methane through undecane, ethylene, propylene, nitrogen, carbon dioxide and hydrogen sulfide. For components in the mixture which are not included in the list, interaction parameters will be calculated from component critical properties and acentric factor. Water is assumed to be immiscible for this option. Computational time is similar to BWRK option. References 7a-d, 8 a-b.

**NOTE:** BWRK and BWRSK have corresponding enthalpy options, BWRH and BWRSH. They are **not** interchangeable. Use BWRH with BWRK and BWRSH with BWRSK.

## CHAO

This method uses a combination of regular solution theory for activity coefficients and empirical functions to describe the liquid phase with the Redlich-Kwong equation for the vapor phase. The correlation was developed for hydrocarbons and hydrogen and should give reasonable values from 60 F to 500 F ( $.5 < Tr < 1.3$ ) for pressures up to about 2000 PSIA ( $P < 0.8 P_c$ ). This option cannot handle components such as CO<sub>2</sub>, H<sub>2</sub>S, or N<sub>2</sub>. Water is assumed to be immiscible for this option. Do not use this technique to model separation of close-boiling components (e.g. ethylene-ethane splitter). Reference 1.

## ESSO

Curve-fitted equations (developed at Exxon Research and Engineering Co.) from the Maxwell-Bonnett vapor pressure charts which are used for heavy hydrocarbon systems (crude oils). Vapor pressures for components 1-8, 10, 11, 22-26, 62, 65 and 68 (Pure Component Data Base ID numbers) are calculated using Figure API8A1.14, page 8-29, American Petroleum Institute. The Curl-Pitzer vapor pressure correlations are used for all other pure substances. This technique is considered an "industry standard" for calculating K-values for heavy hydrocarbons at pressures below 50 PSIA. Water is assumed to be immiscible for this option. Reference 9.

## ESSO TAB

This is a faster, tabular form of the ESSO correlation (vapor pressure charts from the API Technical Data Book). Primarily used for heavy hydrocarbon systems at pressures below 50 PSIA. Water is assumed to be immiscible for this option. Reference 9.

## GERG2008K

GERG (Groupe Européen de Recherches Gazières) 2008 is a wide-range reference equation of state for natural gases and other mixtures (limited to [21 components](#)) based upon a multi-fluid mixture model approximation explicit on the reduced Helmholtz free energy. The [GERG-2008 equation](#) is valid in the gas phase, in the liquid phase, in the supercritical region and for the vapour-liquid equilibrium (VLE). [Range of validity and estimated uncertainty](#). Please note that GERG2008 is a very slow executing equation of state. Reference [GERG-2008](#).

## KVAL

This correlation is based on data for methane systems and can be used for natural gas processes where methane is the predominant component for temperatures between 100F and -300 F (e.g. nitrogen rejection, cryogenic expander plants). This option can also be used for modeling refrigerated lean oil absorbers. Water is assumed to be immiscible for this option.

## LKPK

This is an application of the BWR equation by Lee-Kesler-Ploecker. They use the BWR equation to represent a simple fluid (based on argon, krypton, and methane) and a reference fluid (octane). Mixture calculations use mixture rules, reduced temperature, reduced pressure, and acentric factors to combine simple and reference fluids together. This mixing rule appears to be applicable to mixtures whose components differ appreciably in molecular size, such as synthesis gas from coal or heavy petroleum feedstocks. Binary constants calculated by Ploecker, Knapp, and Prausnitz for a large number of binary pairs containing light gases are included. See *Thermodynamics Table 4. Lee-Kesler Binary Interaction Parameters* for an alphabetical list of the pairs for which a constant is included. Water is assumed to be immiscible for this option. Reference 10.

## MOD ESSO

This is the Lee-Kesler modification to the ESSO vapor pressure correlation. This option should improve prediction of K-values for heavy and aromatic hydrocarbons (Watson characterization factor which is not equal to 12). Water will be assumed to be immiscible for this option. References 9 and 13.

## PENK

The Peng-Robinson equation (without interaction parameters) improves the applicability of the cubic equation of state for vapor-liquid equilibrium calculations in the vicinity of the critical region. With interaction parameters, this option is suitable for simulating cryogenic ethane and propane recovery, nitrogen rejection and systems where H<sub>2</sub>S and CO<sub>2</sub> predominate. Due to the improved universal critical compressibility factor, the Peng-Robinson equation typically gives better results for equilibrium phase composition and critical region calculations than SOAVE or RKK. To improve accuracy further, you can incorporate binary interaction parameters into the calculations either by regression of VLE data via ChemTran or by use of the DESIGN II BINary PARAmeter file PENG 1. See *Thermodynamics Table 3. Peng Robinson Binary Interaction Parameters* for a list of the binary pairs for which VLE data has been regressed. This K-value option may be used to regress equilibrium data (CHEMtran FILE required). If no data is fitted, K-values are generated from the equation of state.

## Chapter 7

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Water is assumed to be immiscible in the PENK option. If you require water to be treated as a miscible component when using the PENK option you should enter **NO IMM** in the GENeral section. This is the default K-value option. Reference 14a.

### PPRK

The Predictive Peng-Robinson correlation enhances the characterization of highly non-ideal systems over a wide range of temperature and pressure. It is generalized as a linear function of acentric factor used for the prediction of liquid densities for heavy hydrocarbons and polar components. Twu et al's (References 56-62) approach on infinite-pressure cubic equations of state mixing rules are used to explain various complex mixture behavior via their new excess Gibbs function.

All available mixture parameters can be calculated from existing UNIFAC data and when needed RENon-NRTL parameters (via ChemTran) can also be used to predict the phase equilibria of all binaries, whether components are polar, nonpolar, inorganic gases and combinations thereof. The Predictive Peng-Robinson equation typically gives better results for equilibrium phase composition and densities than SOAVE or PENK. To improve accuracy further, you can incorporate binary interaction parameters into the calculations either by regression of VLE data via ChemTran using RENon-NRTL or by using internally stored liquid-liquid interactions generated via UNIFAC database of group contributions from each species. Water is assumed to be immiscible in the PPRK option. If you require water to be treated as a miscible component when using the PPRK option you should enter **NO IMM** in the GENeral section. References 54-62.

**NON IDEAL** = i, j, k,...

Enter only the component ID numbers separated by commas that are to be treated as non-ideal in the GENeral section. The command INFinite DILution must be entered with this command.

**INFinite DILution** = i, j, k,...

Enter only the component ID numbers separated by commas that are to be treated at infinite dilution in the GENeral section. The command **NON IDEAL** must be entered with this command.

### REFPROP

REFPROP is an acronym for REFerence fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

At this time, only 57 components are supported but other pure components can be easily added in the future on request. The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>" to use this option.

Reference: Lemmon, E.W., Huber, M.L., McLinden, M.O. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties -REFPROP, Version 8.0, National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2007.

**Other related keywords are as follows:**

#### REFPROP-AGAK

This command makes use of the AGA 8 K-value method built-in REFPROP by NIST.

#### REFPROP-DEFAULTK

This command makes use of the default K-value method built-in REFPROP by NIST.

#### REFPROP-GERGK

This command makes use of the GERG K-value method built-in REFPROP by NIST.

#### REFPROP-PENGROBK

This command makes use of the Peng Robinson K-value method built-in REFPROP by NIST.

### RKK

Redlich-Kwong equation of state with interaction coefficients for CO<sub>2</sub> and H<sub>2</sub>S developed by G. W. Wilson is a cubic equation of state which can be used to model light hydrocarbon mixtures such as cryogenic ethane and propane recovery containing moderate amounts of CO<sub>2</sub> and H<sub>2</sub>S (3-10%) with better success than other options except APISOAVEK or PENK which may have binary interaction parameters. Water is assumed to be immiscible for this option. Reference 16.

### SKDK

The Soave-Kabadi-Danner Technique is particularly suitable for two and three phase equilibrium calculations for water-hydrocarbon systems. The Soave-Kabadi-Danner method is based upon a modified Soave-Redlich-Kwong equation of state. This method applies only to hydrocarbon-water systems. If water is not present in the system, then the SKDK method defaults to APISOAVEK. For accurate predictions of three phase separation, the MULTIPLE PHASE flash module must be used. For all other units, the immiscible water flash method described in the Method of Calculation description for Water K-values in Hydrocarbon Systems in this section is used. The correlation was developed for hydrocarbons up to C<sub>10</sub> and should give reasonable results at up to 550 degrees F. Caution should be used in applying this method to hydrocarbons heavier than C<sub>10</sub> or close to the three phase critical point. SKDK gives better results and is applicable over a wider range of temperatures than the UNIFAC correlation. A group contribution method is used to determine interaction parameters for the following class of hydrocarbons. If a hydrocarbon in your system is not in one of these classes, use of the SKD method is not recommended.

Homologous Series, Alkanes, Alkenes, Dialkenes, Acetylenes, Naphthenes, Cycloalkenes and Aromatics. For non-hydrocarbons, interaction parameters default to zero. References 3a - c.

### SOAVEK

The Soave modification of the Redlich-Kwong cubic equation of state is most typically used for light hydrocarbon systems from cryogenic temperatures to 900F (or below the critical temperature of the mixture) for pressures up to 1000 PSIA. It should be used with caution for pressures greater than 600 PSIA. VLE data can be regressed using the ChemTran program. This K-value option may be used to regress equilibrium data (CHEmtran FILE required). If no data is fitted, K-values are generated from the equation of state. Water is assumed to be immiscible for this option. References 3a and 16.

## Petrochemical and Chemical Industry Recommended K-value Options

Water, unless otherwise specified by the user, receives no special treatment when using the K-values listed below. If water is present in your simulation, you can enter the IMM = 62 in the GENERAL section if you want water treated as an immiscible component (62 is the component ID number for water) or fit data to model water rigorously.

The name on the left is the appropriate keyword spelling for the K-value options. A description of the technique is given on the right. The default K-value option is STDK.

### LL UNIFACK

A group contribution theory developed by J.M. Prausnitz, et.al. and extended by A. Fredenslund, et.al. It generates estimates of the nonideal interactions between binary pairs of components based on the "groups" contained in each component. The UNIFAC model used to predict liquid-liquid phase behavior is the same as that used to predict vapor-liquid equilibrium (UNIFACK). However, the interaction parameters are different. UNIFAC LLE group interactions are available for 32 different groups representing hydrocarbons, water, alcohols, organic acids, and other compounds. To specify the LLE UNIFAC parameter library, the command LLE UNIFAC=1 should be given in addition to the LL UNIFACK command. The correlation is considered accurate for temperatures between 10 and 40 C. This method should be used with caution because it is only an estimation technique. If accuracy is of primary importance, LLE data should be regressed using ChemTran. If water is specified as immiscible (IMM=62), program will force the equation to treat water as miscible component. Reference 20a, 20g.

### MOD PENK

Design II modifications of Peng-Robinson equation of state based on work by Stryjek et al. This equation is applicable for non-ideal chemical systems at high pressure. This method predicts the liquid phase with the accuracy of activity coefficient methods. Its advantages are its improved ability to predict vapor pressures for polar and associating compounds and an improved ability to regress VLE data. This model can be used at pressures higher than those for which the vapor phase can be assumed to be ideal. Use of an Equation of State MIXing rule is recommended. Choices are shown below. The same mixing rule must be used in both DESIGN II and ChemTran. A CHEmtran FILE is required. Please see **ChemTran: MODified PENG K Method** for specific commands and details of this correlation. If no CHEmtran FILE is specified, or Kappa parameters are missing, this method will default to PENK. Reference 14b.

#### EOS MIX = STD

Use the standard symmetric mixing rule (default)

#### EOS MIX = MAR

Use the Margules non-symmetric mixing rule.

#### BIN PAR = TEG1

Use of this command in GENERAL section of the input file will allow users to access TEG/Water/Hydrocarbons binary interaction parameters when Modified Peng Robinson method is used. ChemTran file is no longer required for this mixture system.

### REN

Also known as the Non-Random Two-Liquid equation (NRTL), this is an activity coefficient correlation for modeling non-ideal systems which can be partly or totally miscible. Vapor phase fugacities are calculated using Redlich-Kwong equation of state. This equation has a non-randomness parameter (C12) which makes it applicable to a large variety of mixtures (CHEmtran FILE recommended). This option should only be used if VLE and/or LLE data has been regressed. Without data regression, this equation is very similar to the VAPor PREssure technique. Reference 15.

### UNIFACK

A group contribution theory developed by J.M. Prausnitz, et.al. and extended by A. Fredenslund, et.al. It generates estimates of the non-ideal interactions between binary pairs of components based on the "groups" contained in each component. Approximately 32 groups, such as methyl, hydroxyl, butyl, etc. are available. The correlation is considered accurate for temperatures between 30 and 125 C, and pressures between 1 and 3 atmospheres. All components in the mixture should be condensable (no CO, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, etc.). An example using UNIFACK and LL UNIFAC is at end of this section. Reference 20a-d.

**NOTE:** UNIFACK may be used with non-database components which have been defined in ChemTran using the STRUcture command.

### ZERO UNIFACK

Some simulations will include chemical groups that are not handled by the UNIFACK correlation.

Depending on the concentration and strength of interaction of the uncorrelated chemical groups, UNIFACK may still yield accurate results when the interaction of these chemical groups are ignored. When this command is included in the GENERAL section of the DESIGN II file and/or ChemTran file, the simulation will not halt when an uncorrelated chemical group is encountered. Use of this command depends on good judgment in evaluating the relative interaction of the uncorrelated chemical groups.

When running a ChemTran file, all chemical groups are tabulated and the binary interaction parameters are reported.

## Chapter 7

Parameter values of "zero" indicate uncorrelated chemical groups.

### UNIQUACK

The UNiversal QUAsi-Chemical equation can correlate vapor-liquid equilibrium data for partially and totally miscible systems. The UNIQUAC equation extends the Guggenheim theory of quasi-chemical representation for liquid mixtures by introducing Q (molecular volume) and R (molecular area) parameters and utilizes the Wilson concept of local composition. The main advantage of the UNIQUAC equation is its ability to represent both VLE and LLE with only two adjustable parameters per binary. It is applicable to non-electrolyte mixtures containing non-polar and polar liquids, including those that are involved in hydrogen bonding (CHEmtran FILE required). Vapor phase fugacities are calculated using Redlich-Kwong equation of state. This option should only be used if VLE and/or LLE data has been regressed. Without data regression, this equation is very similar to the VAPor PREssure technique. Reference 21a and b.

### WILSON

The Wilson equation is an activity coefficient equation used for modeling non-ideal, miscible mixtures. (CHEmtran FILE recommended). Vapor phase fugacities are calculated using Redlich-Kwong equation of state. This option should only be used if VLE and/or LLE data has been regressed. Without data regression, this equation is very similar to the VAPor PREssure technique. Reference 23.

### IDEAL VAP

Vapor phase fugacity coefficients are set equal to one. Liquid phase non-ideality is modeled by RENon, WILson, UNIQUAC or UNIFAC as specified by the user (CHEmtran FILE is recommended, except for UNIFAC).

Two options are available for use with the liquid activity coefficient correlations (REN, WIL, UNIQUACK) for modeling vapor-phase association. Both of these methods require CHEmtran FILES for regression of equilibrium data and for entry of dipole moment, parachor, and association parameter for the pure components.

### HADen OCOnnell VAPor

Sets up a virial equation for the calculation of the vapor phase fugacity. The virial equation is of the form  $z = 1 + BP/RT$  where z is the compressibility factor for the vapor, B is the second virial coefficient for the vapor, P is the pressure, R is the molar gas constant, and T is the temperature. The second virial coefficients are calculated by the method of Hayden and O'Connell. Reference 50.

### CHEmical THEory VAPor

Sets up a virial equation for the calculation of the vapor phase fugacity but adds a model that represents strongly associating chemicals in the vapor phase. A chemical equilibrium is established to represent the formation of dimers and cross dimers that form in the vapor phase with these types of chemicals. Hayden and O'Connell methods are used to calculate the equilibrium constants for the formation of dimers and Nothnagel's formulations are used to account for these equilibria. (Reference 51).

### Ideal or Tabular K-value options

Water, unless otherwise specified by the user, receives no special treatment when using the K-values listed below. If water is present in your simulation, you can enter the IMM = 62 in the GENeral section if you want water treated as an immiscible component (62 is the component ID number for water) or fit data to model water rigorously.

The name on the left is the appropriate keyword spelling for the K-value options. A description of the technique is given on the right. The default K-value option is STDK.

### IDEALK

Liquid phase activity coefficients are set equal to one and vapor phase fugacity coefficients are calculated using the Redlich-Kwong equation. This option will differ from VAPor PREssure calculations as temperature and/or pressure increases.

### TABK

Tabular or interpolative K-values versus Temperature data can be entered for any or all components via a CHEmtran FILE. The three equations available are:  $(K/T)^{1/3} = A + BT + CT^2 + DT^3$ ,  $\ln K = A + B/T + C/T^2$ ,  $\ln KP = A + B/T + C/T^2$

Where: K is the equilibrium constant  
T is the absolute temperature  
P is the pressure  
A, B, C & D are the constants

$$(K/T)^{1/3} = A + BT + CT^2 + DT^3$$
$$\ln K = A + B/T + C/T^2$$
$$\ln KP = A + B/T + C/T^2$$

A temperature range is specified for the tabular data in ChemTran. For conditions outside that range, the K-value technique specified in the GENeral section is used.

For interpolative K versus T data, both temperature and pressure range are specified, and several sets can be entered for each component via a CHEmtran FILE. Linear interpolation is done between points specified in the data sets if the temperature and pressure are within the specified ranges. If the temperature or pressure is outside the interpolative data ranges, the K-value technique specified in the GENeral section is used.

You should always specify a K-value technique to be used when temperature and/or pressure are outside the range of your tabular/interpolative data. (CHEmtran FILE required).

TABular K-values are entered via a CHEmtran FILE for individual components with K-Ti = commands. The tabular K-values for these components override the K-value option specified in the GENeral section or individual equipment modules.

Note: Added the capability to allow only the specific module to use TABK via "equipment specific tabular" K-value usage. Commands required are:

1. In general section **TABK EQU** which stands for **TABK EQUIPMENT** specific.
2. In equipment which uses the above Chemtran generated K-values via KEYK = TABK. The components for which tabular K-values are entered will have their global option values over written by the tabular K-values for this equipment. But for all other equipments on the file only the chosen global thermodynamic method values will be calculated.

## VAP PRE

K-values are based on the standard data base correlation for pure component vapor pressures. This option is primarily used for low pressure separations where liquid phase interactions are ideal. For components not in the PURE COMPONENT DATA BASE, ChemTran can be used to predict or correlate vapor pressure data.

## Special K-value options

Water is assumed to be totally miscible for these options, even if user specifies water as immiscible.

## AMINEK

Rigorous model for removal of CO<sub>2</sub> and/or H<sub>2</sub>S from natural gas streams using MEA, DEA, MDEA, DGA, and DIPA amine solutions. Please see *Thermodynamics Table 6. Mixed Amine Modeling* for other components for which this technique is applicable. K-values for all components are calculated using Kent-Eisenberg and Deshmukh-Mather models. Both models contain parameters that have been fitted to experimental vapor-liquid equilibrium data for single-acid gas (carbon dioxide or hydrogen sulfide), single-amine systems. The liquid-phase reactions are linked to the vapor phase through Henry's law physical-solubility relationships for carbon dioxide and hydrogen sulfide in water. Solution nonidealities are accounted for in a pragmatic way by fitting the equilibrium constant for the amine protonation reaction using experimental hydrogen sulfide data and fitting the carbamate formation reaction constant to experimental carbon dioxide data. Regressed coefficients are available for MEA, DGA, DEA, DIPA and MDEA.

**Note:** Piperazine addition is also possible into the AMINEK method. The effect of Piperazine on CO<sub>2</sub> removal has been researched in detail since 1992 (references 1 & 2 below). From the conclusions that both research groups have published, MDEA-piperazine system is a promising solvent for CO<sub>2</sub> removal. It is claimed that a solvent of piperazine/MDEA (5 wt. %/45 wt. %) provides almost two orders of magnitude and more enhancement in sour gas absorption than a 50 wt. % MDEA at low loading and one order of magnitude enhancement at moderate loading (mole of gas/mole of amine).

1. G.-W. Xu, Zhang C.-F, S.-J. Qin, and Y.-W. Wang, Kinetics study on absorption of carbon dioxide into solutions of activated methyl diethanolamine, *Industrial & Engineering Chemistry Research* 31 (1992), 921-927.
2. S. Bishnoi and G.T. Rochelle, Absorption of carbon dioxide into aqueous piperazine: reaction kinetics, mass transfer and solubility, *Chemical Engineering Science* 55 (2000), 5531-5543.

## APISOUR

Sour water systems containing hydrogen sulfide, ammonia, carbon dioxide and water can be accurately modeled using this technique. K-values for hydrogen, nitrogen, methane, ethane, propane, iso-butane, and normal butane which are dissolved in the aqueous solution are calculated by Henry's law. Addition of caustic (sodium or potassium hydroxide) and organic acids (formic, acetic, propionic, or butyric) to control the pH and therefore the solubilities of NH<sub>3</sub>, H<sub>2</sub>S, and CO<sub>2</sub> in water can also be modeled. Note that reactions are **not** allowed by adding strong acids to precipitate salts.

K-values for hydrocarbons heavier than n-butane are calculated based on the n-C<sub>4</sub> Henry's constant. All other components will have K-values computed from the Chao-Seader correlation. Data used for this correlation for ammonia covers concentrations from 1 ppm to 30 weight percent, temperatures ranging from 20 C to 140 C and pressures up to 200 PSIA. Acid gas concentration data ranges from 0.0 to 4.0 moles of acid gas per kilogram of solution for either H<sub>2</sub>S or CO<sub>2</sub>. A pH range from 2 to 14 is handled. Reference 5.

## DMPEGK

This equation can be used to model the removal of acid gases such as CO<sub>2</sub>, H<sub>2</sub>S, COS, and mercaptans from natural and synthesis gas systems with DMPEG, a physical solvent that is a mixture of polyglycols. DMPEG is also known by the trade names such as Coastal AGR, Selexol and Genosorb 1753. DESIGN II contains the necessary pure component data for DMPEG (component ID no. 1218) to calculate k-values, enthalpies and viscosities. Allowed components for DMPEGK are listed in [Thermodynamics Table 2. DMPEG Solvent absorption modeling](#). Among the species H<sub>2</sub>S and methyl mercaptan has a highest solubility in DMPEG than CO<sub>2</sub> does, making DMPEG selective for H<sub>2</sub>S or mercaptan removal. References 63, 64, 65 and 66.

## EDWARDK

K-values for weak, aqueous electrolytic solutions based on the Edwards et al., model. The solvent must be water. Total solute concentrations should be  $\leq 10$  molal (gram moles of solute per kilogram of solvent) and total ionic strength should be less than or equal to 6 molal. Henry's total constants are required for all solutes in water. *Thermodynamics Table 5. Henry's Constants in Water List* contains a list of Henry's constants in water which are available with this model. The user must specify ionic species and reactions using the IONIC COMponents and LIBrary REACTIONS commands. If user defined ions and reactions are present, a CHEMtran FILE is required. References 19b-f.

## EPSOURK

## Chapter 7

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K-values for weak, aqueous electrolytic solutions based on the Edwards et al., model. This method is applicable for all ions, reactions, and components which are in the Design II ionic library. *Thermodynamics Table 5. Henry's Constants in Water List* contains the list of components for which Henry's constants in water are available. References 19b-f.

### MDEAK

Rigorous model for removal of CO<sub>2</sub> and/or H<sub>2</sub>S from natural gas streams using either monoethanolamine (component ID no. 4155) or diethanolamine (component ID no. 4051) solutions. Other components for which this technique is applicable include methane, ethane, ethylene, propane, propylene, iso-butane, normal butane, 1 butene, cis-2 butene, trans-2 butene, 1,3 butadiene, carbon monoxide, nitrogen, carbonyl sulfide, and hydrogen. K-values for hydrocarbons heavier than n-butane are calculated based on the n-C<sub>4</sub> Henry's constant. All other components will have K-values computed from the Chao-Seader correlation. Components which do not appear in this list should be combined with the components which they most closely resemble, because STDK is used to predict K-values for all other components. STDK tends to overstate the solubilities of components in the amine solution. You can override the Chao-Seader K-values by entering your own K-T data via ChemTran. References 12a - c.

### SOURK

Sour water strippers can be handled accurately using the Beychok method. NH<sub>3</sub>, H<sub>2</sub>S and H<sub>2</sub>O interaction data is provided automatically. If the ratio of ammonia to hydrogen sulfide is outside the range of 1.5 to 20, or your system contains CO<sub>2</sub>, you should use the APISOUR option. Reference 19.

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## Thermodynamics: Selecting K-Value Options

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**NOTE:** Water should be specified as immiscible for hydrocarbon systems.

For most light hydrocarbon systems above 60 F, the standard Chao-Seader option could be used. For temperatures below 60F, SOAVEK's could be used. If methane makes up at least 75% of the hydrocarbons in a natural gas stream and the temperatures are between 100 F and -300F, KVAL should be considered (LNG and Natural Gas Expander Plants). For heavy hydrocarbons at pressures below 50 PSIA the ESSO charts (API data book) can be used. For systems for which vapor-liquid equilibrium data are available, Peng-Robinson can be used and VLE data utilized via CHEMTRAN.

Care must be taken with all techniques when non-hydrocarbon components, such as H<sub>2</sub>S, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, CO, and NH<sub>3</sub>, appear in the process. Aromatics and naphthenic components in lean or crude oils can also have significant compositional effects on light hydrocarbon K-values. These systems can be handled most accurately by entering vapor-liquid equilibrium data via ChemTran or by using an appropriate BIN PAR file.

For processes where you wish to use more than one technique, you can specify different K-values for different equipment modules using the KKEY command described in each equipment module section.

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## Thermodynamics: Relative Speed of K-Values

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All K-value calculation techniques are fairly fast with the exception of Redlich-Kwong, Wilson, Renon, Peng-Robinson, BWRS, APISOUR, and Uniquac. Redlich-Kwong and Peng-Robinson are about twice as slow as the fast techniques. The others mentioned above are about five times slower.

## Thermodynamics: Enthalpy Options

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### Thermodynamics: Enthalpy (H) and Entropy (S) Options

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Care must be taken when modeling systems for which the heat of mixing is significant. You can regress excess enthalpy data via ChemTran to improve prediction of this behavior. For processes where you wish to use more than one technique, you can specify different enthalpies for different equipment modules using the HKEY command described in each equipment module section.

**NOTE:** For non-standard components (ID numbers 100-199, 200-299), the values that you enter for the acentric factor or ideal gas heat capacity are important in the calculation of enthalpies.

#### Gas Processing and Petroleum Refining Recommended Enthalpy options

(choose one of the following options)

The name on the left is the appropriate keyword spelling for the enthalpy options. A description of the technique is given on the right. The default enthalpy option is PENH.

#### STDH

This method uses a combination of regular solution theory for activity coefficients and empirical functions to describe the liquid phase with the Redlich-Kwong equation for the vapor phase. The standard enthalpy technique can be used for most natural gas applications with little sacrifice in accuracy (5-15%). Extra care should be taken for temperature below -100F and for pressures greater than 2000 PSIA. Reference 16.

#### API

Also known as the Grayson-Johnson equation, this option can be used to model heavy hydrocarbon enthalpies. Reference 24a.

## APIMOD

A modification to the Grayson-Johnson enthalpy technique improves predictions for high pressure regions, particularly near the critical regions. Reference 24b.

## APISOAVEH

The American Petroleum Institute has generated interaction parameters for H<sub>2</sub>S, CO<sub>2</sub>, CO, and N<sub>2</sub> with several hydrocarbons to be used with the SOAVE equation of state. A special function is used to treat hydrogen in these mixtures. For components not in *Thermodynamics Table 1. APISOAVEK Interaction Parameter List.*, DESIGN II will use a component's solubility parameter to estimate binary interaction parameters with H<sub>2</sub>S, CO<sub>2</sub>, or N<sub>2</sub> for the SOAVE equation. References 3a and 4.

## BWRH

This is an application of the Benedict-Webb-Rubin equation of state. It is an eleven parameter equation developed for light hydrocarbon mixtures containing methane through pentane, nitrogen and carbon dioxide in the range of 26 to 400 F. The BWRH enthalpy option is normally used with the BWRK K-value option. This is a very slow option. References 7a-d.

## BWRSH

This is an application of the 11 parameter Benedict-Webb-Rubin equation of state by Starling, et. al. It has an extended list of interaction coefficients and generalized correlation for parameters by Starling. It is very accurate for hydrocarbon mixtures containing methane through undecane, ethylene, propylene, nitrogen, carbon dioxide, and hydrogen sulfide. It is also very slow. The BWRSH enthalpy option is normally used with the BWRSK K-values option. References 7a-d, 8a-b.

## COPE

The corresponding states enthalpy and entropy technique is extremely accurate for light hydrocarbon systems. Temperatures as low as -300 F and pressures as high as 6000 PSIA can be handled. COPE is very slow. You should consider using another enthalpy option for rigorous column simulations before the final design run is to be made. References 26a and b.

## CURI-pitzer

This enthalpy technique uses the three-parameter corresponding states principle proposed by Pitzer and co-workers. Volumetric and thermodynamic properties have been correlated in tabular form for non-polar substances over the range of reduced temperatures, 0.8 to 4.0, and reduced pressures, 0.0 to 9.0. This correlation should not be used in the critical region, for liquids at low temperatures or for widely boiling mixtures, particularly those which contain high concentrations of very light and very heavy components. With the CURL enthalpy technique, you can choose one the MIXing RULEs to evaluate pseudocritical properties and acentric factors of mixtures. References 27a-d.

## GERG2008H

GERG (Groupe Européen de Recherches Gazières) 2008 is a wide-range reference equation of state for natural gases and other mixtures (limited to [21 components](#)) based upon a multi-fluid mixture model approximation explicit on the reduced Helmholtz free energy. The [GERG-2008 equation](#) is valid in the gas phase, in the liquid phase, in the supercritical region and for the vapour-liquid equilibrium (VLE). [Range of validity and estimated uncertainty](#). Please note that GERG2008 is a very slow executing equation of state. Reference [GERG-2008](#).

## GRAYson-Johnson

See API enthalpy option.

## LEE

Lee and Kesler modified the CURL-Pitzer enthalpy equation to extend the temperature range to  $0.3 < T_r < 4.0$  and the pressure range to  $0 < P_r < 10$ . This correlation should be more accurate than the CURL option for calculations near the critical region or at low temperatures. The LEE option allows you the choice of MIXing RULEs as described above for CURL. Reference 31.

## LEEMOD

This method is a modification of the Johnson and Grayson equation for petroleum applications by Lee and Kesler. It is correlated using specific gravity and Watson K factor. API, API MOD, and LEE MOD are simple equations and are not as accurate as equation of state methods. Reference 25

## LKPH

This is an application of the BWR equation by Lee-Kesler-Ploecker. They use the BWR equation to represent a simple fluid (based on argon, krypton, and methane) and a reference fluid (octane). Mixture calculations use mixture rules, reduced temperature, reduced pressure, and acentric factors to combine simple and reference fluids together. This mixing rule appears to be applicable to mixtures whose components differ appreciably in molecular size, such as synthesis gas from coal or heavy petroleum feedstocks. Binary constants calculated by Ploecker, Knapp, and Prausnitz for a large number of binary pairs containing light gases are included. See *Thermodynamics Table 4. Lee- Kesler Binary Interaction Parameters* for an alphabetical list of the pairs for which a constant is included. Reference 10.

## PENH

The Peng-Robinson cubic equation of state (without interaction parameters) is used to calculate vapor and liquid enthalpies. This is one of the more accurate techniques for natural gas mixtures, particularly in the critical or retrograde region. Reference 14.

## PPRH

The Predictive Peng-Robinson is used to calculate vapor and liquid enthalpies. This uses non-ideal liquid phase interactions via UNIFAC by default and RENon, if mixture data is regressed via ChemTran. References 54-62.

## REFPROPH

## Chapter 7

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REFPROP is an acronym for REFerence fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

At this time Helium is supported along with 56 other pure components. The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>" to use this option.

Reference: Lemmon, E.W., Huber, M.L., McLinden, M.O. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties -REFPROP, Version 8.0, National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2007.

**Other related keywords are as follows:**

### **REFPROP-AGAH**

This command makes use of the AGA 8 enthalpy method built-in REFPROP by NIST.

### **REFPROP-DEFAULTH**

This command makes use of the default enthalpy method built-in REFPROP by NIST.

### **REFPROP-GERGH**

This command makes use of the GERG enthalpy method built-in REFPROP by NIST.

### **REFPROP-PENGROBH**

This command makes use of the Peng Robinson enthalpy method built-in REFPROP by NIST.

### **RKH**

The Redlich-Kwong cubic equation of state is used to calculate vapor and liquid enthalpies. This option differs from STDH in that binary interaction parameters for CO<sub>2</sub> and H<sub>2</sub>S with light hydrocarbons are included. This option can be very slow. References 16 and 33.

### **SKDH**

The Kabadi-Danner modification of the Soave-Redlich-Kwong equation of state calculates enthalpies for hydrocarbon-water systems. References 3a-c.

### **SOAVEH**

The SOAVE modification of the Redlich-Kwong equation of state is used to predict enthalpies. Primarily used for natural gas mixtures over a wide range of temperatures and pressures. Occasional convergence difficulties may occur in rigorous distillation columns at high (close to critical) pressures. Use STDH to get reasonable temperature profile. References 3a and 16.

### **MIXing RULE =**

1. Kay's rule (the fastest, also the default). Reference 28
2. Stewart, Burkhart and Voo's rule. Reference 29
3. Leland and Mueller's rule. Reference 30
4. Lee and Kesler's rule. Reference 31

**NOTE:** These mixing rules are for use with the CURL and LEE enthalpy methods. Mixing rules 2 and 3 are extremely slow.

### **Petrochemical and Chemical Recommended Enthalpy Options**

#### **LATent heat**

Liquid enthalpies will be calculated from latent heat data from the PURE COMPONENT DATA BASE. Vapor enthalpies will be calculated using the Redlich-Kwong equation of state. The LATent heat equation does not take into account liquid heat of mixing. This technique is primarily used for non-ideal mixtures at low to moderate pressures.

#### **EXCess plus LATent heat**

Excess enthalpy (heat of solution or mixing) data can be input through ChemTran as a function of temperature and liquid composition. This data can then be used with latent heat type enthalpies. This option should be used for alcohol-water or acid-water systems. When excess enthalpy data is not available, RENON constants reduced from binary VLE data can be used to calculate the excess enthalpy via ChemTran. (CHEmtran FILE required).

#### **EXCess plus TABular**

Excess enthalpy data entered via ChemTran can also be used with tabular liquid and vapor enthalpies. (CHEmtran FILE required).

#### **MOD PENH**

Design II modification of Peng-Robinson equation for enthalpies based on work by Stryjek et al. Reference 14b.

#### **YEN**

This technique can be used to calculate liquid enthalpies for non-ideal processes which do not exhibit substantial heats of solution or mixing (excess enthalpy data should be entered via ChemTran instead). Vapor enthalpies will be calculated using STDH. This enthalpy option does not contain a pressure correction term. Use of this enthalpy option is not recommended for systems containing valves and other processes that produce a pressure drop. Reference 34.

#### **Ideal and Tabular Enthalpy Options**

The name on the left is the appropriate keyword spelling for the enthalpy options. A description of the technique is given on the right. The default enthalpy option is STDH.



## IDEALH

Ideal gas heat capacity and tabular liquid enthalpy data is entered via ChemTran for every component in your simulation. (CHEmtran FILE required).

## TABH

Tabular vapor and liquid enthalpies versus temperature can be entered via ChemTran. Tabular values must be entered for all components in a mixture if they are entered for any component. (CHEmtran FILE required).

## Special Enthalpy Options

The name on the left is the appropriate keyword spelling for the enthalpy options. A description of the technique is given on the right. The default enthalpy option is PENH.

## AMINEH

Treating of natural gas with MEA, DEA, MDEA, DGA, and DIPA amine solutions involve gas-liquid interface thermodynamics. The Peng-Robinson equation is used to calculate the enthalpy of the gas phase. For the liquid phase, a modified polynomial fit to amine-gas data is used.

## DMPEGH

This technique predicts enthalpies for acid gas removal of CO<sub>2</sub> and H<sub>2</sub>S using the physical solvent DMPEG. The heat of absorption of the allowed components in DMPEG is automatically handled when available. See [Thermodynamics Table 2. DMPEG Solvent absorption modeling](#) for those components that will be modelled using DMPEG. References 63, 64, 65 and 66.

## EDWARDH

Enthalpy option based on Edwards et al., to be used with weak aqueous electrolyte systems containing user defined ions and reactions. If any ions, reactions or components are not in the pure component database, a CHEmtran FILE is required. Reference 19b-e.

## EPSOURH

Enthalpy option to be used for weak, aqueous electrolytic systems for which all ions, reactions, and components are in the Design II pure component database. May also be used with APISOUR. Reference 19b-e.

## LIQCP

This method is specifically used for only liquid mixtures. It may be used for systems with negligible vapor in the mixture. By default, STDH is used for the vapor portion of the vapor/liquid mixture. It will use mole fraction mixing rules for calculating the enthalpy of the mixture from the individual component enthalpies. An excess enthalpy correction is made for Glycol-Water (ID#62) systems, where glycols can be one among Ethylene Glycol (ID# 3103); Di-Ethylene Glycol (ID# 4030); Tri-Ethylene Glycol (ID# 4044); Propylene Glycol (ID#4031). A liquid heat transfer fluid, THERMINOL 55-ID#2055 & THERMINOL 66-ID#2054 (copyrights Solutia Inc.) can also use this method for heat exchanger calculations.

**WARNING:** LIQCP method should not be used for mixtures with vapor phases.

## MDEAH

Sweetening of natural gas with monoethanolamine (MEA) or diethanolamine (DEA) involves chemical reactions. The heats of solution for CO<sub>2</sub> and H<sub>2</sub>S are handled automatically by this technique. Reference 32a-d.

## Thermodynamics: Enthalpy Datum

The enthalpy of a gas in its ideal state (very low pressure, but customarily measured at 1 ATM) and 32 F is set to zero. This means most liquid enthalpies and vapor enthalpies at low temperatures will be reported as negative numbers.

NOTE: These datum is for molecules, not elements, so the datum is different for products and reactants such as in reactors.

## Thermodynamics: Selecting Enthalpy Option

Typically, the enthalpy option corresponding to the selected K-value option can be used. COPE is more accurate for most light hydrocarbon systems and should be used when pressures are above 100 PSIA and temperatures are below -100F. COPE is slow and should not be used for rigorous column calculations unless necessary for the final designs. LATent heat or YEN Alexander enthalpy options should be considered for chemicals systems. API, API MOD, CURL, and LEE are enthalpy techniques appropriate for heavy hydrocarbon systems.

## Thermodynamics: Density Options

The density calculation is defaulted to Yen Woods (STDD) option. In most cases, a chosen K-value and Enthalpy method has a corresponding Density method available and unless the user selects the matching option, STDD will be used by default. For instance, when APISOAVEK/APISOAVEH is specified, unless the user selects APISOAVED, the default STDD density option will be used. SOAVE liquid densities are often 10 to 15% in error and another density selection should be made. For streams containing more than 10% (by weight) heavy hydrocarbon components, IDEALD or STDD should be considered.

**Note:** With V9.30, users can use a different liquid density method for any of the options given below by using the following command in the GENERAL section (or via Specify...Basic Thermo dialog)

The name on the left is the appropriate keyword spelling for the density options. A description of the technique is given on the right.

## Chapter 7

**DEN LIQ** = Enter symbolic name for Density option. (e.g. DEN LIQ = PEND)

### STDD

Default option. The Yen-Woods correlation for calculating liquid densities is formed from two contributions. The first contribution gives the density of the liquid at its saturation pressure. The second contribution corrects for deviation from saturated conditions. Yen Woods is an improved analytical form of the original tabular corresponding states method of Lydersen, Greenkorn and Hougen. Predictions of petroleum fraction densities have been improved. The vapor phase densities are calculated using the Redlich-Kwong cubic equation of state. A mixing rule option is available for Yen Woods density option for calculation of critical properties.

**YEN WOODS MIX = KAY** (default) or **RK**

The mixing rule options are Kay and Redlich-Kwong. The RK method estimates the critical parameters by finding the values of  $T_c$  and  $V_c$  that satisfy the critical point conditions for the Redlich-Kwong equation of state. For all systems, the new RK option will give a better estimate of critical properties than the KAY option. However, KAY will generally yield valid results when the ratio of the largest  $P_c$  to the smallest  $P_c$  is less than 2.0 and the ratio of the largest  $T_c$  to the smallest  $T_c$  is less than 2.0. References 16, 28.

**Note:** STDH uses the STDD calculations while determining liquid enthalpies. Changing the mixing rule can affect enthalpy calculations also.

Standard volumes and densities for the first 63 components in the pure component database are calculated from the gallons per lbmol value in the database. The Rackett correction for different NTP/STP conditions is applied. All other components use the Yen Wood method. Add a STD VOL-YEN command if you want the Yen Woods method used for the first 63 components instead. References 16 and 35.

### AGAD

The American Gas Association density correlation was developed for natural gas mixtures. Its primary applications are for prediction of natural gas densities, metering of natural gas and estimation of gas reservoir reserves. This method is generally applicable for compositions within the following range:

<u>Component</u>	<u>Mole Percent</u>
Methane	50-100 %
Nitrogen	0-50
Carbon Dioxide	0-50
Ethane	0-20
Propane	0-5
Butane	0-3
Pentane	0-2
Hexane and heavier	0-1
Water vapor, H <sub>2</sub> S, H <sub>2</sub> , CO, O <sub>2</sub> , Helium and Argon	0-1

Tests indicate that the method predicts densities for both liquid and vapor accurately even beyond stated composition ranges. While this method can be used at pressures above 20,000 psia and temperatures above 400 degrees F, results should be viewed with caution and reduced accuracy should be expected. Reference 35a.

### AMINED

Liquid molar volumes are calculated using the Rackett equation and Amagat's Law.

### APISOAVED

Soave densities with API interaction parameters. The API version of the SOAVE cubic equation of state is used to calculate vapor and liquid densities. Liquid densities for hydrocarbon streams may be 10-15% in error. References 3 and 4.

### BWRD

This is an application of the Benedict-Webb-Rubin equation of state. It is an eleven parameter equation developed for light hydrocarbon mixtures containing methane through pentane, nitrogen and carbon dioxide in the range of 26 F to 400 F. The Benedict-Webb-Rubin equation of state (11 parameter) is used to calculate vapor and liquid densities. The calculation is based on density data and can be very slow. References 7a-d.

### BWRSD

This is an application of the 11 parameter Benedict-Webb-Rubin equation of state by Starling, et. al. It has an extended list of interaction coefficients and generalized correlation for parameters by Starling. The calculation is based on density data, and calculations can be very slow. References 7a-d and 8a and b.

### COPEd

The corresponding states density technique is based on density data. Results for density for light hydrocarbon and non-condensables such as H<sub>2</sub>S, CO<sub>2</sub>, and N<sub>2</sub> should be very accurate, but calculations can be slow. References 26a and b.

### COSTALD

Liquid density calculation for pure compounds and mixtures is more accurately made using the correlation COSTALD-CORresponding STAtes Liquid Density than other accepted procedures. COSTALD is based on 6,338 density data points for pure, nonpolar liquids, 1,352 points for polar and quantum liquids, and 6,926 mixture density points including 319 points for LNG/LPG mixtures. COSTALD accurately predicts the densities for saturated and compressed liquid and liquid mixtures for temperatures in the general range of 50 to 600 K and pressures from saturation to 68,950 KPa (10,000 psia) using only critical temperature, critical pressure, SRK acentric factor, saturated liquid volume, and saturation pressure. The vapor phase densities are calculated using the Redlich-Kwong cubic equation of state without interaction parameters.

References 28 a, b, and 16.

## GERG2008D

GERG (Groupe Européen de Recherches Gazières) 2008 is a wide-range reference equation of state for natural gases and other mixtures (limited to [21 components](#)) based upon a multi-fluid mixture model approximation explicit on the reduced Helmholtz free energy. The [GERG-2008 equation](#) is valid in the gas phase, in the liquid phase, in the supercritical region and for the vapour-liquid equilibrium (VLE). [Range of validity and estimated uncertainty](#). Please note that GERG2004 is a very slow executing equation of state. Reference [GERG-2008](#).

## IDEALD

The mixture density is calculated from the pure component liquid volumes as follows:

$$\rho_{\text{mix}} = 1/x_i V_i$$

where  $x_i$  are mole fractions and  $V_i$  is calculated either from the characteristic volume equation or from V-T data entered in ChemTran. The characteristic volume equation is:

$$VW = (V/5.7 + 3.0 Tr)$$

where  $V$  is the liquid molar volume in cm<sup>3</sup>/gmol at the atmospheric boiling point and  $Tr$  is the boiling point divided by the critical temperature, in degrees Kelvin. No volume change due to mixing is assumed. The Redlich-Kwong cubic equation of state is used to calculate vapor densities.

## LKPD

This is an application of the BWR equation by Lee-Kesler-Ploecker. They use the BWR equation to represent a simple fluid (based on argon, krypton, and methane) and a reference fluid (octane). Mixture calculations use mixture rules, reduced temperature, reduced pressure, and acentric factors to combine simple and reference fluids together. This mixing rule appears to be applicable to mixtures whose components differ appreciably in molecular size, such as synthesis gas from coal or heavy petroleum feedstocks. Binary constants calculated by Ploecker, Knapp, and Prausnitz for a large number of binary pairs containing light gases are included. See *Thermodynamics Table 4. Lee-Kesler Binary Interaction Parameters* for an alphabetical list of the pairs for which a constant is included. Reference 10.

## MOD PEND

The Modified Peng-Robinson cubic equation of state is used to calculate vapor and liquid densities. Reference 14b.

## PEND

The Peng-Robinson cubic equation of state (without interaction parameters) is used to calculate vapor and liquid densities. This technique models critical/retrograde region better for light hydrocarbon systems than any of the cubic equations of state except the BWR options. Reference 14a.

## PPRD

The Predictive Peng-Robinson is used to calculate vapor and liquid densities. This uses non-ideal liquid phase interactions via UNIFAC by default and RENon, if mixture data is regressed via ChemTran. References 54-62.

## REFPROP

REFPROP is an acronym for REFerence fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>"

Reference: Lemmon, E.W., Huber, M.L., McLinden, M.O. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties -[REFPROP](#), Version 8.0, National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2007.

**Other related keywords are as follows:**

### REFPROP-AGAD

This command makes use of the AGA 8 density method built-in REFPROP by NIST.

### REFPROP-DEFAULTD

This command makes use of the default density method built-in REFPROP by NIST.

### REFPROP-GERGD

This command makes use of the GERG density method built-in REFPROP by NIST.

### REFPROP-PENGROBD

This command makes use of the Peng Robinson density method built-in REFPROP by NIST.

## RKD

Redlich-Kwong cubic equation of state (with interaction parameters) is used to calculate vapor and liquid densities. The small increase in accuracy gained using RKK, RKH, and RKD rather than default options may be offset by the relatively large increase in computation time. Reference 16.

## SKDD

Kabadi-Danner modification of Soave-Redlich-Kwong equation of state is used to calculate vapor and liquid densities for hydrocarbon-water systems. References 3a-c.

## SOAVED

## Chapter 7

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Soave modification of Redlich-Kwong equation of state is used to calculate vapor and liquid densities. Soave liquid densities may be 10-15% in error. Peneloux Correction to SOAVED that improves density prediction for known hydrocarbons are automatically included by default. For modifications to these corrections for specific components or for petroleum fractions, please see *Thermodynamics: Peneloux Correction to Soave Density* for specific commands to use. Reference 3a, 3d and 16.

**NOTE:** An enthalpy option specified in an equipment module with the HKE = command does not change the density option. Use the DKE = command if you also want a different density option for that module calculation.

### Thermodynamics: Transport Property Options

The viscosity, thermal conductivity, and surface tension of mixtures are important properties in most sizing or rating calculations. DESIGN II has several calculation options for each of these properties. They are:

The option for viscosity, thermal conductivity, and surface tension will be set based on the presence of any of the following in your input:

- **REF**ine module,
- **CRU**de feed section,
- **PET**roleum **STR**eam command

Heat exchanger rating calculations for streams which are steam or cooling water will use STEam TABLEs automatically for all thermophysical properties.

Otherwise the default viscosity and thermal conductivity option is NBS81 and the default surface tension option is STD. You may, of course, override the program defaults by entering the appropriate keyword commands.

#### Transport Properties

##### TRANSport =

Enter option for calculating viscosity and thermal conductivity. Default is NBS81. However, if a CRUde section is present, then API becomes the default.

The name on the left is the appropriate keyword spelling for the transport property options. A description of the technique is given on the right.

##### NBS81

A corresponding states technique developed by Ely and Hanley of the Thermophysical Properties Division of the National Bureau of Standards, this method predicts reasonable values for vapor and liquid viscosities for real and pseudo-components up to boiling points of approximately 1000F. Reference 36.

##### API

The American Petroleum Institute techniques for calculating vapor and liquid viscosities. One technique predicts viscosities based on mixture gravities and Watson K-factor, the other relies on user-provided viscosity curve data. Reference 37a.

##### TWU

The Twu method is an internally consistent method for the calculation of liquid viscosities of petroleum fractions. The liquid viscosities are predicted based on n-alkanes as reference fluid and employs normal boiling point and specific gravity. Viscosities of petroleum fractions with normal boiling point up to 1800 R and API gravity up to -30 can be predicted, which is within the practical region of interest. API method is used for vapor viscosities. Reference 38b.

##### LNAV

Data for thermal conductivity and viscosity are available for many components in the PURE COMPONENT DATA BASE. These are temperature dependent curves which are suitable for use at low pressures or at pressures which are not too different from the mixture saturation pressure. LNAV represents the following equation:

$$\ln(\text{mixture property}) = \sum x_i (\ln \text{property } i)$$

where "i" is the component ID number and  $x_i$  is the mole fraction of "i".

You may also enter thermal conductivity and viscosity data for components via *ChemTran* and fit the data to the LNAV equation.

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### Thermodynamics: Viscosity Options

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You may select a separate method to calculate viscosity independent of the method used to calculate thermal conductivity.

##### VIScosity =

Enter option for viscosity calculation. Default is NBS81. However, if a CRUde section is present, then API becomes the default.

##### VIScosity of VAPor=

Enter this command for a specific vapor viscosity method. Default is NBS81. However, if a CRUde section is present, then API becomes the default.

##### VIScosity of LIQuid=

Enter this command for a specific liquid viscosity method. Default is NBS81. However, if a CRUde section is present, then

API becomes the default.

(choose one of the following options)

## AMINE

Liquid phase viscosity is calculated using DIPPR Procedure 8H with corrections based on experimental data for the effects of amine type, strength and gas loading. For gas mixtures, the Brokaw method for polar gases is used with the Dean-Stiel correction for high pressure.

## DEAN

The Dean and Stiel technique was designed to predict vapor viscosities. The liquid viscosities predicted by this technique can be in considerable error. Reference 38a.

## EXC MOL VI

A new liquid excess molar viscosity method for binary mixtures.

## TWU

The Twu method is an internally consistent method for the calculation of liquid viscosities of petroleum fractions. The liquid viscosities are predicted based on n-alkanes as reference fluid and employs normal boiling point and specific gravity. Viscosities of petroleum fractions with normal boiling point up to 1800 R and API gravity up to -30 can be predicted, which is within the practical region of interest. Dean-Stiel method is used for vapor viscosities. Reference 38b.

## API

The American Petroleum Institute techniques for calculating liquid viscosities. One method predicts viscosities based on mixture gravities and Watson K-factor, the other relies on user-provided viscosity curve data. Vapor viscosities predicted by this method can be in considerable error. If you let the viscosity default to API, use Dean-Stiel vapor viscosities. Reference 37a.

## NBS81

A corresponding states technique developed by Ely and Hanley of the Thermophysical Properties Division of the National Bureau of Standards, this method predicts reasonable values for vapor and liquid viscosities for real and pseudo-components up to boiling points of approximately 1000F. Reference 36.

## LNAV

Data for thermal conductivity and viscosity for PURE COMPONENT DATA BASE. These are temperature dependent curves which are suitable for use at low pressures or at pressures which are not too different from the mixture saturation pressure. LNAV represents the following equation:

$$\ln(\text{mixture property}) = \sum X_i (\ln \text{property } i)$$

where "i" is the component ID number and xi is the mole fraction of "i".

## MIX2

This method is used to predict gas mixture viscosity. MIX2 represents the following equation: Viscosity of mixture =  $\{\sum X_i * \text{Viscosity}(i) * (\text{Molecular weight } i)^{1/2}\} / \{\sum X_i * (\text{Molecular weight } i)^{1/2}\}$

where "i" is the component ID number and xi is the mole fraction of "i". Reference 38c.

## MODAPI

Specifies revised API method for liquid and vapor viscosities. Reference 37b.

## REFPROP

REFPROP is an acronym for REFerence fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

At this time Helium is supported along with 56 other pure components. The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>". Reference 64.

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## Thermodynamics: Thermal Conductivity Options

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You may select a separate method to calculate thermal conductivity independent of the viscosity calculation method. Pure component vapor phase thermal conductivities are calculated using the API method (Reference 42) and thermal conductivity for vapor mixtures are calculated by the Wassiljewa equation (Reference 42b). These calculation are in effect when the following thermal conductivity method is specified: **TEMA new**, **TEMA Old**, or **API**.

### THErmal CONductivity =

Enter option for calculating thermal conductivity. Default is NBS81. If the simulation contains a CRUde section, then default is TEMA new.

### THErmal CONductivity VAPor=

Enter option for calculating vapor thermal conductivity. If the simulation contains a CRUde section, then default is TEMA new.

### THErmal CONductivity LIQuid=

Enter option for calculating liquid thermal conductivity. If the simulation contains a CRUde section, then default is TEMA new.

(choose one of the following options)

## Chapter 7

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### AMINE

For ideal gases, DIPPR method for pure components is used. For gases at low to moderate pressure, the Wassiljewa-Mason-Saxena method is used. At high pressure, the Stiel-Thodos method is used. DIPPR methods are used for liquids. References 42b and 42c.

### NBS81

This is a corresponding states technique for predicting thermal conductivities for liquid mixtures which was developed by Ely and Hanley of the Thermophysical Properties Division of the National Bureau of Standards (under partial sponsorship of the Office of Standard Reference Data). Reference 36.

### TEMA new

Tubular Exchangers Manufacturers Association technique calculates liquid thermal conductivity as a function of both temperature and API gravity of the liquid. Vapor phase thermal conductivities are calculated using the API method for pure components Wassiljewa equation for mixture calculations. References 40a-d.

### Tema Old

Tubular Exchangers Manufacturers Association technique calculates thermal conductivity as a function of liquid temperature. Vapor phase thermal conductivities are calculated using the API method for pure components and the Wassiljewa equation (Ref 42b) for mixture calculations. References 39 and 40b-d.

### API

The American Petroleum Institute technique calculates thermal conductivity as a function of liquid temperature. Vapor phase thermal conductivities are calculated using the API method (Ref 42) for pure components and the Wassiljewa equation (Ref 42b) for mixture calculations.

### LNAV

Data for thermal conductivity and viscosity are available for many components in the PURE COMPONENT DATA BASE. These are temperature dependent curves which are suitable for use at low pressures or at pressures which are not too different from the mixture saturation pressure. LNAV represents the following equation:

$$\ln(\text{mixture property}) = \sum x_i (\ln \text{property } i)$$

where "i" is the component ID number and  $x_i$  is the mole fraction of "i".

LI Calculation of thermal conductivity using the method of Li. Reference 41.

### MIX3

This method is used to predict gas mixture thermal conductivity. MIX3 represents the following equation: Thermal conductivity of mixture =  $\{\sum x_i \cdot \text{Thermal Conductivity } (i) \cdot (\text{Molecular weight } i)^{1/3}\} / \{\sum x_i \cdot (\text{Molecular weight } i)^{1/3}\}$

where "i" is the component ID number and  $x_i$  is the mole fraction of "i". Reference 42a.

### REFPROP

REFPROP is an acronym for REFERENCE fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

At this time Helium is supported along with 56 other pure components. The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>". Reference 64.

---

## Thermodynamics: Surface Tension Options

---

You may select a separate method to calculate surface tension independent of the method used to calculate viscosity and thermal conductivity.

### SURface TENSION =

Enter option for calculating surface tension. Default is STD. However, if a CRUDE section is present, the default is API. (choose one of the following options)

### API

Surface tension for liquids is calculated using techniques of the American Petroleum Institute. This method includes estimation of surface tension for the heavy hydrocarbon (petroleum fractions) cuts. Reference 42.

### REFPROP

REFPROP is an acronym for REFERENCE fluid PROPERTIES. This program, developed by the National Institute of Standards and Technology (NIST), provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons, especially natural gas systems.

At this time Helium is supported along with 56 other pure components. The user must have the REFPROP DLL installed on their PC in order to use the method. If the REFPROP DLL is not installed, the following message will be displayed: "ERROR: Could not find INFO dll in " "c:\program files\refprop\refprop.dll. Please purchase "REFPROP from NIST at <http://www.nist.gov/srd/nist23.htm>". Reference 64.

### STD

Surface tension for liquids is calculated using a molar average of surface tension for individual components.

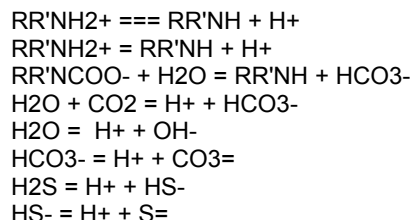
## Thermodynamics: Mixed Amine

Mixed Amine thermodynamics can be used for the steady-state modeling of gas treating operations for carbon dioxide and hydrogen sulfide removal using aqueous solutions of a variety of amines. Primary application areas are refinery operations, natural gas processing, chemicals production, syngas treating, flue gas processing and fuel conversion processes.

### Thermodynamics: Mixed Amine Models

Mixed Amine K-value option offers two thermodynamic models: Deshmukh-Mather (DESH) and Kent-Eisenberg (KENT). Both models contain parameters that have been fitted to experimental vapor-liquid equilibrium data for single-acid-gas (carbon dioxide or hydrogen sulfide), single-amine systems.

Both models are based on the following reaction equilibria:



where R and R' represent alcohol groups.

#### Thermodynamics: Kent-Eisenberg Model (KENT)

The Kent and Eisenberg model (Hydrocarbon Processing, 55, 87-92 [1976]) is a unit activity coefficient model in which the equilibrium constants, K, for the reactions are correlated by  $\ln(K)$  versus a polynomial in  $1/T$ .

The liquid-phase reactions are linked to the vapor phase through Henry's law physical-solubility relationships for carbon dioxide and hydrogen sulfide in water.

Solution nonidealities are accounted for in a pragmatic way by fitting the equilibrium constant for the amine protonation reaction using experimental hydrogen sulfide data and fitting the carbamate formation reaction constant to experimental carbon dioxide data.

Regressed coefficients are available for MEA, DGA, DEA, DIPA and MDEA using the "Mixed Amine" option.

#### Thermodynamics: Deshmukh-Mather Model (DESH)

This model, due to Deshmukh and Mather (Chem.Eng.Sci., 36, 355-362 [1981]), is based on the extended Debye-Hückel theory for weak electrolytes and the framework established by Edwards et al. (AIChE Journal, 24, 966 [1968]).

The extended Debye-Hückel expression used for the prediction of activity coefficients is the form used by Guggenheim and Stokes (Trans. Far. Soc., 54, 1646 [1958]) and Scatchard (J. Am. Chem. Soc., 83, 2636 [1961]) for concentrated solutions:

$$\ln \gamma_j = \frac{-2.303A * z_j^2 \sqrt{I}}{1 + B\sqrt{I}} + 2 \sum \beta_j * m$$

Here 'A' is the Debye-Hückel limiting slope (0.509 at 25C in water), 'B' is a temperature-dependent constant, 'I' is ionic strength, 'm' is molality; 'z' is the ionic charge, and the  $\beta$ 's are two-body interaction parameters.

The first term represents the contribution from electrostatic forces and the second accounts for short range van der Waals forces. This equation represents the nonideality of solutions of weak electrolytes quite well while retaining a computationally simple form.

The Deshmukh-Mather model has been fitted to all public-domain data for the solubility of CO<sub>2</sub> and H<sub>2</sub>S in aqueous solutions of MEA, DGA, DEA, DIPA and MDEA and has been used with excellent results to predict proprietary experimental data for gas solubility in solvent mixtures.

Currently, mixed amine thermodynamics contains one set of methods for calculating all the necessary physical properties, "Mixed Amine".

### Thermodynamics: Mixed Amine Notes

When Mixed Amine thermodynamics is chosen the following simulation criteria are essential and should be followed:

- You MUST enter TWO AMINES into the component list.
- Handles up to 40 total number of components or less in a simulation problem.
- The standard components are: H<sub>2</sub>O, TWO Amines, H<sub>2</sub>S, and CO<sub>2</sub>; and you can supply up to fifteen additional components.
- All the components selected must be one among the 45 components in the Component Database for Mixed Amine.

## Chapter 7

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- If one of the selected components is MDEA, enter it as the second amine in the components list; using it in this order increases the stability of the calculations.
- You can use Mixed Amine for systems containing a single amine also. When prompted for concentration on the amines, enter zero as the concentration for one. The report program includes the extra amine in all stream and column component information and will show very small (non-zero) values of its concentration.
- A flowsheet converges best if the circulation rate and amine concentration are specified on the same stream and this stream is one of the tear (recycle) streams.
- Rich-end pinched columns (absorbers producing very heavily loaded solutions and over-boiled strippers) tend to converge much more slowly than columns limited by VLE (pinched) at the lean end.
- Entropy calculations are not performed for Mixed Amine systems. This applies to equipment modules selected for performing entropy calculations. Some are pumps, flash, and compressors.

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### Thermodynamics: Mixed Amine Physical Properties

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Mixed Amine contains one set of methods for calculating all the necessary physical properties. The following physical and transport properties models are used:

**EQUATION OF STATE** - Peng-Robinson equation is used for the gas phase.

**ENTHALPY** - The Peng-Robinson equation is used to calculate the enthalpy of the gas phase. For the liquid phase, a modified polynomial fit to data is used.

**ACTIVITY COEFFICIENTS** - Liquid phase activities are taken to be unity in the Kent-Eisenberg model or they are calculated using an extended Debye-Hückel equation in the Deshmukh-Mather model.

**LIQUID MOLAR VOLUME** - Liquid molar volumes are calculated using the Rackett equation and Amagat's Law.

**VAPOR PRESSURE** - The vapor pressure of pure components is calculated using the Antoine equation.

**HENRY'S COEFFICIENTS** - Henry coefficients are calculated using a polynomial fit to experimental solubility data in water, corrected for concentration of the amine and for ionic strength effects.

**HEAT CAPACITY** - Design Institute for Physical Property Research (DIPPR) methods are used for the liquid phase. For the vapor phase, ideal gas heat capacities are used along with the Reid, Prusnitz, and Sherwood (RPS) correction.

**HEATS OF REACTION** - Reaction heat is calculated for some reactions using polynomial fits to reduced phase equilibrium data and in other cases by direct thermodynamic calculation using an activity coefficient model.

**HEATS OF SOLUTION** - Polynomial fit to reduced thermodynamic data.

**VISCOSITY** - Liquid phase viscosity is calculated using DIPPR Procedure 8H with corrections based on experimental data for the effects of amine type, strength and gas loading. For gas mixtures, the Brokaw method for polar gases is used with the Dean-Stiel correction for high pressure. References 42d & 42e,

**DIFFUSION COEFFICIENTS** - Modified polynomial fit for CO<sub>2</sub> in water with Barret's equation for temperature corrections. For H<sub>2</sub>S in water, the Haimor-Sandall relation is used; this is adjusted for amine concentration through a viscosity correction.

The diffusion coefficient of amines in water is determined using the Hikita-Ishikawa-Uku-Murakami equation. The diffusion coefficient of CO<sub>2</sub> in amines is calculated from the Barret equation for water, corrected for amine concentration using the data and equation of Blauwhoff, Versteeg and van Swaaij.

Diffusion coefficients of components in the gas phase are calculated using the Fuller-Schettler-Giddings equation when the gas is essentially non-polar as is the case in most absorbers. For polar gases, generally in regenerators where the water content is high, the Chapman-Enskog-Wilke-Lee-Brokaw equation is used.

**THERMAL CONDUCTIVITY** - For ideal gases, DIPPR method for pure components is used. For gases at low to moderate pressure, the Wassiljewa-Mason-Saxena method is used. At high pressure, the Stiel-Thodos method is used. References 42b & 42c.

**SURFACE TENSION** - A DIPPR polynomial is used for pure components and the results applied to mixtures using a weighted sum of components contributions.

**OTHER PARAMETERS** - Other pure-component parameters such as critical constants, molecular weights compressibility factors, acentric factors, dipole moments and so on are calculated using the data bank of Reid, Prausnitz and Sherwood, 'The Properties of Gases and Liquids', 3rd Edition, pp. 629 - 665, McGraw-Hill Book Co., New York, 1977.

### Thermodynamics: Pure Component Property Commands

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#### Thermodynamics: Critical Properties and Acentric Factor Specification

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At any time, additional thermophysical data for a particular component may be provided directly to DESIGN II for simulation calculation. The provided data will be used rather than allowing DESIGN II to estimate properties for the components specified. The critical properties (T<sub>c</sub>, P<sub>c</sub>, V<sub>c</sub>) and acentric factors( $\omega$ ) may be entered in the GENeral section of DESIGN II



input. DESIGN II will use this data in subsequent calculations. The commands for entering this information are:

(select any of the following commands)

**TC** (T units) i =

Enter critical temperature of component "i" in the specified units or default input units.

**PC** (P units) i =

Enter critical pressure of component "i" in the specified units or default input units.

**VC** (L3 units/molar Q units) i =

Enter critical volume of component "i" in the specified units.

**ACE** i =

Enter acentric factor for component "i".

**Example:**

Enter a critical temperature of 600F and a critical pressure of 23 atm for component 12.

**TC 12 = 600, PC (ATM) 12 = 23**

## Thermodynamics: Data Factors Tc, Pc, MW Calculation Options

### Critical Temperature, Critical Pressure and Molecular Weight

DESIGN II allows using the following commands when the simulation contains PETroleum fractions or CRUde feed section.

#### Critical Temperature Estimation Options

**DATa TC KEY** =

Enter option for prediction of critical temperature for petroleum fractions. Default option is CAVett.

(choose one of the following options)

**CAVett**

This is the default correlation for calculating critical temperatures for petroleum fractions. Reference 44.

**COAL** liquids

Correlation developed by Wilson, et.al for estimating critical temperatures for petroleum fractions, especially those with Watson characterization factors which are less than 11. Reference 43.

**LEE**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions. References 25 and 31.

**NOKay**

Method for calculating critical pressure for paraffinic, olefinic, naphthenic and aromatic hydrocarbons with boiling points in the range of -40 to 1000F and specific gravities in the range of 0.5 to 1.0. Reference 45.

**WATson**

The Lee-Kesler technique is used to calculate critical temperatures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31, and 43.

#### Critical Pressure Estimation Options (choose one of the following options)

**DATa PC KEY** =

Enter option for prediction of critical pressure for petroleum fractions. Default option is CAVett.

**CAVett**

This is the default correlation for calculating critical pressures for petroleum fractions. Reference 44.

**COAL** liquids

Correlation developed by Wilson, et.al. for calculating critical pressures for petroleum fractions, especially those with Watson characterization factors which are less than 11. References 43.

**HERZog**

Method for estimating critical pressure using vapor pressure, boiling points and parachors for substances. Works best for saturated and unsaturated hydrocarbons; accuracy decreases for aromatic and cyclic compounds. Reference 46.

**LEE**

Lee-Kesler technique is used to calculate critical pressures for petroleum fractions. References 25 and 31.

**WATson**

The Lee-Kesler correlation is used to calculate critical pressures for petroleum fractions with Watson characterization factors greater than 11. References 25, 31 and 43.

#### Molecular Weight Estimation Option (choose one of the following options)

**DATa MOL KEY** =

Enter option for prediction of molecular weight for petroleum fractions. Default option for petroleum fractions entered in GENERAL section is CAVett. Default option for CRUde feed description is HARIu.

**CAVett**

This is the default option for predicting molecular weight when petroleum fraction commands are entered in the GENERAL

## Chapter 7

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section (AMB i =, API i =). Reference 44.

### API

Technique developed by M. Riazi at the Pennsylvania State University for calculating molecular weights of petroleum fractions. This technique should be avoided for light hydrocarbons (hexanes and lighter). Reference 48.

### HARiu

This is the default option for predicting molecular weights for petroleum fractions if you use any of the following in your simulation: REFine module, CRUDE feed section or PETroleum STReam print option. Reference 47.

### LEE

Lee-Kesler correlation for calculating molecular weights for petroleum fractions. Reference 25 and 31.

---

## Thermodynamics: Heating Value Specification

---

You can override the default heating value which DESIGN II will calculate for the petroleum fraction components by entering a HIGH HEATING value or LOW HEATING value command for each petroleum fraction. The heating value calculated by DESIGN II for petroleum fraction components can also be adjusted by entering your own value for the CARBON to HYDROGEN weight ratio for each petroleum fraction. You can also use these commands to enter heating values for component in the Pure Component Data Base

The methods used by DESIGN II to obtain heating values and carbon-to-hydrogen ratios are based on general correlations. Greater accuracy in the calculations can be obtained by using laboratory-derived high or low heating values or carbon/hydrogen ratios.

(choose any of the following options)

### HIGH HEATING value (H units/molar Q units) i =

Enter desired high (wet) heating value for petroleum fraction "i", where "i" is the component ID number. High heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with liquid water formed by the reaction.

### LOW HEATING value (H units/molar Q units) i =

Enter desired low heating value for petroleum fraction "i", where "i" is the component ID number. The low heating value is defined as the change in enthalpy resulting from the combustion of a substance at atmospheric pressure, beginning and ending at a temperature of 60 F, with water remaining in the gaseous state.

### CARBON to HYDROGEN weight ratio i =

Enter the desired value for petroleum fraction "i", where "i" is the component ID number. The heating value calculated by DESIGN II for petroleum fraction components CARBON to HYDROGEN weight ratio for each petroleum fraction. The default value will be calculated using Figure 2B2.1 from the API *Technical Data Book*.

Be sure to enter at least four significant figures for the CAR HYD command as this value can affect the mass balance in reactor calculations.

---

## Thermodynamics: Heat of Formation and Entropy of Formation Specification

---

The LOST work calculation (thermodynamic efficiency of a process) requires heat of formation and entropy of formation for each component in the process when a reactor module (REA, EQU REA, PLU, REA, CSTR, etc.) is used. In addition, for calculations which include any REACTOR module, both the heat of formation and entropy of formation for all components in the system must be known before its calculations can be performed. Heats of formation and entropies of formation for component ID numbers 1 through 99 are automatically available from the Pure Component Data Base. Temperature basis for heat and entropy of formation values is 25 C. References 53a-c.

You can use the following commands to specify appropriate values for other components:

### HEAT of FORMATION (H units/molar Q units) i =

Enter the heat of formation for component "i", where "i" is the component ID number.

### HEAT of FORMATION LIQUID (H units/molar Q units) i =

Enter the heat of formation on a liquid basis for component "i", where "i" is the component ID number.

### ENTROPY of FORMATION (H units/molar Q units/T units) i =

Enter the entropy of formation for component "i", where "i" is the component ID number.

**NOTE:** The ENTROPY of FORMATION command allows five sets of unit options. They are as follows:

BTU/LBMOL/R (default)      CAL/GMOL/K      KCAL/KGMOL/K      KJ/KGMOL/K      J/GMOL/K

### Example:

```
GENeral
COMPONENTS = 2,49,48,62,1021
HEAT of FORMATION (BTU/LBMOL) 1021 = - 86544
ENTROPY of FORMATION (BTU/LBMOL/R) 1021 = - 30.9901
```

---

## Thermodynamics: Peneloux Correction to Soave Density

---

The Peneloux Correction to SOAVED can be modified by including the following command in the GENeral section or under Specify...Keyword Input.

**PNA FRA 100** =0.9,0.1,0.0,10

where 100 = is the component ID number  
 0.9 = is the volume fraction of paraffin based component.  
 0.1 = is volume fraction of Naphthene based component.  
 0.0 = is volume fraction of Aromatic based component  
 10.0 = is the number of carbon atoms in the molecule.  
 If not entered, program calculates the value.

This optional command is used to correct the density calculated using SOAVED. If not given for petroleum fractions default values of Paraffins=0.7, Naphthenes=0.2, Aromatics=0.1, and calculated carbon number will be used. Component database contains the needed data for most standard components such as hydrocarbons. However, accuracy will be diminished for non-hydrocarbons (except usual light gases).

- NOTE:** 1. The command can also be used for any component including non-standard components. Reference 3d.  
 2. The Peneloux Corrections for all existing components are stored in the DESIGN II database components.

## Thermodynamics: Property Command Summary

### ChemTran Files and Data Libraries

**CHE**mtran **FILE** = *name1,name2,name3*  
**BIN**ary **PAR**ameters = **PENG1**  
**PET**roleum **BIN**ary **PAR**ameter = **GPA1**

### Water K-Values in Hydrocarbon Systems

**IMM**iscible =  
**GPA WAT**er  
**SOL**ubility of **WAT**er = **COM**ponent  
**NO IMM**iscible

### Equilibrium Constants (K-values) Commands

#### Gas Processing and Petroleum Refining

<b>STDK</b>	<b>CHAO</b> -Seader	<b>MOD ESSO</b>
<b>AMINEK</b>	<b>ESSO</b>	<b>PENK</b> (Peng-Robinson) - DEFAULT
<b>APISOAVEK</b>	<b>ESSO TAB</b>	<b>REFPROP</b>
<b>BRAUN</b>	<b>GERG2004K</b>	<b>RKK</b> (Redlich-Kwong)
<b>BWRK</b>	<b>KVAL</b>	<b>SOAVEK</b>
<b>BWRSK</b>	<b>LKPK</b> (Lee-Kesler)	<b>STDK</b>

#### Petrochemical and Chemical

<b>REN</b> on	<b>UNIFACK</b>	<b>WIL</b> son
<b>IDEAL VAP</b>	<b>UNIQUACK</b>	<b>ZER</b> o <b>UNIF</b> ack

#### Ideal or Tabular values

<b>IDEALK</b>	<b>TABK</b>	<b>VAP PRE</b>	<b>TABK</b>
---------------	-------------	----------------	-------------

#### Special Options

<b>APISOUR</b>	<b>AMINEK</b>	<b>MDEAK</b>	<b>SOURK</b>
----------------	---------------	--------------	--------------

### Enthalpy (H) and Entropy (S) Options

#### Gas Processing and Petroleum Refining

<b>STDH</b>	<b>BWRH</b>	<b>LEE</b>
<b>AMINEH</b>	<b>BWRSH</b>	<b>LKPH</b>
<b>API</b>	<b>COPE</b>	<b>PENH</b> (Peng-Robinson) - DEFAULT
<b>APIMOD</b>	<b>CURI</b> -Pitzer	<b>RKH</b> (Redlich-Kwong)
<b>APISOAVEH</b>	<b>GRA</b> yson-Johnson	<b>SOAVEH</b>
<b>MIX</b> ing <b>RUL</b> e = 1, 2, or 3 where		
1 = Kay's rule (default)	2 = Stewart, Burkhart and Voo's rule	3 = Leland and Mueller's rule

#### Petrochemical and Chemical

<b>LAT</b> ent heat	<b>EXC</b> ess <b>LAT</b> ent	<b>EXC</b> ess <b>TAB</b>	<b>YEN</b>
---------------------	-------------------------------	---------------------------	------------

#### Ideal or Tabular

<b>IDEALH</b>	<b>TABH</b>	
---------------	-------------	--

#### Special Options

<b>AMINEH</b>	<b>MDEAH</b>	
---------------	--------------	--

### Density Options

<b>DEN LIQ</b> = (for liquid density only)	<b>COPED</b>	<b>REFD</b>
<b>STDD</b> (default)	<b>COSTALD</b>	<b>RKD</b>
<b>AMINED</b>	<b>IDEALD</b>	<b>SOAVED</b>

## Chapter 7

APISOAVED  
BWRD  
BWRSD

LKPD  
PEND

### Transport Property Options

TRANS = NBS81  
TRANS = API  
TRANS = LNAV  
TRANS = AMINE

### Viscosity Options

VIScosity VAPor =  
VIScosity LIQuid =  
VIScosity = NBS81  
VIScosity = DEAN  
VIScosity = API  
VIScosity = LNAV  
VIScosity = TWU  
VIScosity = AMINE  
VIScosity VAPor = MIX2

### Thermal Conductivity Options

THERmal CONductivity = AMINE  
THERmal CONductivity VAPor =  
THERmal CONductivity LIQuid =  
THERmal CONductivity = NBS81 (default)  
THERmal CONductivity = TEMA new  
THERmal CONductivity = Tema Old  
THERmal CONductivity = API  
THERmal CONductivity = LNAV  
THERmal CONductivity = LI  
THERmal CONductivity VAPor = MIX3

### Critical Properties and Acentric Factor Options

TC (T units) i =  
PC (P units) i =  
VC (L3 units/molar Q units) i =  
ACE i =  
PNA FRA i =

### Critical Temperature Prediction Methods

DATa TC KEY = CAVett  
DATa TC KEY = COAL liquids  
DATa TC KEY = LEE  
DATa TC KEY = NOKay  
DATa TC KEY = WATson

### Critical Pressure Prediction Methods

DATa PC KEY = CAVett  
DATa PC KEY = COAL liquids  
DATa PC KEY = HERZog  
DATa PC KEY = LEE  
DATa PC KEY = WATson

### Data Factors Tc, Pc, MW Calculation Options

DATa MOL KEY = CAVett  
DATa MOL KEY = API  
DATa MOL KEY = HARIu  
DATa MOL KEY = LEE

### Surface Tension Options

SURface TENsion = API  
SURface TENsion = STD

### Petroleum Fractions Heating Value Specification

HIGH HEAting value (H units/molar Q units) i =  
LOW HEAting value (H units/molar Q units) i =  
CARbon to HYDrogen weight ratio i =

### Specifications for Component With ID Numbers > 98

HEAt of FORmation (H units/molar Q units) i =  
HEAt of FORmation (H units/molar Q units) i =  
ENTropy of FORmation (H units/molar Q units/T units) i =

## Thermodynamics: Step by Step

### Thermodynamics STEP 1

#### **Choose optional data library and water K-value options.**

Three names of ChemTran data file separated by commas (names are 1 to 4 alphanumeric characters each)

CHE FIL = name1,  
name2, name3

Name for the set of binary interaction parameters from the DESIGN II library appropriate for thermodynamic options

- PENG1 data library file

BIN PAR = PENG1  
PET BIN PAR = GPA1

- Peng-Robinson data library file for petroleum fractions

#### **Water K-value specification** (enter any of the following four commands)

Component ID number for the component that is to be treated as immiscible (water is treated as a special case)

IMM =

Calculate hydrocarbon vapor phase saturated with water in accordance with the Gas Processors

Suppliers Association chart

GPA WAT

Calculate water solubility in liquid hydrocarbons on a component basis rather than using the default water-in-kerosene calculation

SOL WAT = COM

Treat water miscible when using K-value options that normally assume water-hydrocarbon mixtures are immiscible

NO IMM

### Thermodynamics STEP 2

#### **Choose the appropriate K-value option. Gas processing and petroleum refining recommended K-values (enter keyword)**

Chao-Seader equation with Grayson-Streed modifications (water treated as immiscible)

STDK

Soave equation of state with interaction coefficients for CO, CO<sub>2</sub>, H<sub>2</sub>S AND N<sub>2</sub> (water treated as immiscible)

APISOAVEK

Braun K-10 equation (water treated as immiscible)

BRAUN

Benedict, Webb, Rubin and Starling equation of state using special parameters for light natural gas systems (water treated as immiscible)	BWRK
BWRS equation of state with extended list of interaction coefficients and generalized correlation for parameters by Starling (water treated as immiscible)	BWRSK
Chao-Seader equation (water treated as immiscible)	CHAO
Maxwell-Bonnell vapor pressure K-value equation (water treated as immiscible)	ESSO
Tabular charts for Maxwell-Bonnell vapor pressures (water treated as immiscible)	ESSO TAB
K-value technique based on Rice University data for methane systems (water treated as immiscible)	KVAL
Lee-Kesler-Ploecker equation with interaction parameters for H <sub>2</sub> , CO <sub>2</sub> , H <sub>2</sub> S and other light gases (water treated as immiscible)	LKPK
Lee-Kesler modification of Maxwell-Bonnell vapor pressure technique (water treated as immiscible)	MOD ESSO
Peng-Robinson equation of state without interaction parameters (default; water treated as immiscible)	PENK
Redlich-Kwong equation of state with interaction coefficients for CO <sub>2</sub> and H <sub>2</sub> S developed by G.W. Wilson (water treated as immiscible)	RKK
Soave modification of Redlich-Kwong equation of state (water treated as immiscible)	SOAVEK
Petrochemical and chemical industry recommended K-values (enter keyword)	
<b>NOTE:</b> Water receives no special treatment unless user enters VLE or LLE data for the component interactions with water.	
Renon activity coefficient equation (CHEmtran FILE recommended)	REN
K-values estimated using group contribution technique	UNIFACK
UNIQUACK activity coefficient equation (CHEmtran FILE recommended)	UNIQUACK
Wilson activity coefficient equation (CHEmtran FILE recommended)	WIL
Vapor phase fugacity coefficients set to 1, liquid phase modeled by RENon, WILson, UNIQUAC or UNIFAC as specified by user (CHE FIL recommended for RENon, WILson and UNIQUAC)	IDEAL VAP
<b>Ideal or tabular K-value</b> options (water receives no special treatment)	
Activity coefficient set to 1, Redlich-Kwong fugacity coefficient for the vapor phase	IDEALK
Tabular K-values (CHEmtran FILE required)	TABK
Individual component vapor pressures used to generate K-values (Raoult's Law K-values)	VAP PRE
<b>Special K-value</b> options (water is totally miscible)	
Equation for NH <sub>3</sub> , H <sub>2</sub> S, CO <sub>2</sub> , H <sub>2</sub> O plus caustics/organic acids	APISOUR
Correlation for MEA, DEA, MDEA, DGA, and DIPA, CO <sub>2</sub> , H <sub>2</sub> S, and water system	AMINEK
Equation for mono- or di-ethanolamine CO <sub>2</sub> , H <sub>2</sub> S and water	MDEAK
Beychok technique for NH <sub>3</sub> , H <sub>2</sub> S and water	SOURK

## Thermodynamics STEP 3

Gas processing and petroleum refining recommended enthalpy options. Choose the appropriate enthalpy option.	
Redlich-Kwong equation without binary interactions	STDH
Grayson-Johnson equation	API
Grayson-Johnson equation as modified by Lee-Kesler	APIMOD
Soave equation of state with API Technical Data Book interaction coefficients for CO, CO <sub>2</sub> , H <sub>2</sub> S and N <sub>2</sub> with hydrocarbons	APISOAVEH
Benedict, Webb Rubin and Starling equation of state (recommended if BWRK option specified)	BWRH
BWRS equation of state with extended list of interaction coefficients (recommended if BWRSK option specified)	BWRSH
Corresponding states enthalpy technique	COPE
Curl-Pitzer enthalpy equation (use the MIX RULE command to specify the rule you want DESIGN II to use)	CUR
Grayson-Johnson (API) enthalpies	GRA
Lee-Kesler modification of the Curl-Pitzer enthalpy technique (MIX RUL can be specified)	LEE
Lee-Kesler-Ploecker equation of state with interaction parameters for H <sub>2</sub> , CO <sub>2</sub> , H <sub>2</sub> S and other light gases	LKPH
Peng-Robinson enthalpies without interaction parameters (default)	PENH
Redlich-Kwong enthalpies with interaction parameters	RKH
Soave (modification of Redlich-Kwong) enthalpies	SOAVEH
Optional mixing rule (select one of the following options)	
- Kay's rule (default)	MIX RUL = 1
- Stewart, Burkhart and Voo's rule	MIX RUL = 2
- Leland and Mueller's rule	MIX RUL = 3
Petrochemical and chemical industry recommended enthalpy options	
Vapor enthalpies from the Redlich-Kwong equation and latent heat enthalpies from the Pure Component Data Base	LAT
Excess enthalpy as a function of temperature and liquid composition plus data base latent heat values (CHEmtran FILE is required)	EXC LAT
Excess enthalpy as a function of temperature and liquid composition plus tabular liquid and vapor enthalpies (CHEmtran FILE is required)	EXC TAB
Yen-Alexander liquid enthalpies	YEN
Ideal and tabular enthalpy options	
Ideal Gas with tabular liquid enthalpies (CHEmtran FILE is required)	IDEALH

## Chapter 7

Tabular vapor and liquid enthalpies for all components in the system (CHEmtran FILE is required)	TABH
Special enthalpy options	
Enthalpies for mono- or di-ethanolamine, CO <sub>2</sub> , H <sub>2</sub> O and water systems	MDEAH
Enthalpies for MEA, DEA, MDEA, DGA, and DIPA, CO <sub>2</sub> , H <sub>2</sub> S, and water system	AMINEH

### Thermodynamics STEP 4

#### Density option specification (select ONE of the following options)

Yen-Woods liquid densities, Redlich-Kwong vapor densities (default)	STDD
Densities for MEA, DEA, MDEA, DGA, and DIPA, CO <sub>2</sub> , H <sub>2</sub> S, and water system	AMINED
Soave densities with API interaction parameters	APISOAVED
Benedict, Webb, Rubin and Starling densities	BWRD
BWRS densities with extended list of interaction parameters	BWRSO
Corresponding states densities	COPEO
Corresponding States Liquid Density calculation for pure compounds, saturated and compressed liquid and liquid mixtures.	COSTALD
Ideal liquid densities with characteristic volume temperature correction, Redlich-Kwong vapor densities	IDEALD
Lee-Kesler-Ploecker densities with interaction parameters	LKPD
Peng-Robinson densities without interaction parameters	PEND
Ideal liquid densities with Yen-Woods temperature correction, Redlich-Kwong vapor densities	REFD
Redlich-Kwong densities (with interaction parameters)	RKD
Soave (modification of Redlich-Kwong) densities	SOAVED

### Thermodynamics STEP 5

#### Transport properties specification, choose the appropriate transport property options by selecting either TRANS or VIS AND SUR TEN options

National Bureau of Standards method for calculating viscosity and thermal conductivity	TRANS = NBS81
Transport property for MEA, DEA, MDEA, DGA, and DIPA, CO <sub>2</sub> , H <sub>2</sub> S, and water system	TRANS = AMINE
American Petroleum Institute method for calculating viscosity and thermal conductivity	TRANS = API
Natural log of pure component	TRANS = LNAV

Separate viscosity and thermal conductivity calculation specifications

#### Viscosity of Vapor

VIS VAP =

#### Viscosity of Liquid

VIS LIQ =

Viscosity Calculation method (select ONE of the following SIX options)

- National Bureau of Standards method (default)	VIS = NBS81
- Dean and Stiel method	VIS = DEAN
- Mixed Amine method	VIS = AMINE
- American Petroleum Institute method (default if CRUde section present)	VIS = API
- Natural log of pure component	VIS = LNAV
- Twu viscosity method for the calculation of liquid viscosities of petroleum fractions	VIS = TWU
- Viscosity of Gas Mixture (by Maxwell)	VIS VAP = MIX2

#### Thermal Conductivity of Vapor

THE CON VAP =

#### Thermal Conductivity of Liquid

THE CON LIQ =

Thermal Conductivity calculation method (select ONE of the following SEVEN options)

- National Bureau of Standards method (default)	THE CON = NBS81
- Tubular Exchangers Manufacturers Association new method (default if CRUde section present)	THE CON = TEMA
- Tubular Exchangers Manufacturers Association old method	THE CON = T O
- Mixed Amine Correlation	THE CON = AMINE
- American Petroleum Institute method	THE CON = API
- Natural log of pure component	THE CON = LNAV
- C.C. Li method	THE CON = LI
- C.C. Li method	THE CON VAP=MIX3
- Thermal Conductivity of Gas Mixture (Friend and Adler from Perry's 5 <sup>th</sup> Edition, pp 3-244)	

### Thermodynamics STEP 6

#### Surface tension calculation method. Choose any of the thermal and physical properties options listed below.

#### Primarily used to adjust values estimated for petroleum fractions or petroleum CUTS.

Molar average of surface tension for individual components (default)	SUR TEN = STD
Mixed Amine method	SUR TEN = AMINE
American Petroleum Institute method	SUR TEN = API
Critical properties and acentric factor specification (select any of the following)	
Critical temperature of component "i"	TC (T units) i =

Critical pressure of component "i"	PC (P units) i =
Critical volume of component "i"	VC (T units) i =
Acentric factor for component "i"	ACE i =
Critical temperature prediction method (select ONE of the following five options)	
Cavett method for petroleum fractions (default)	DAT TC KE = CAV
Coal liquids method for petroleum fractions	DAT TC KE = COAL
Nokay method for olefinic, naphthenic and aromatic hydrocarbons	DAT TC KE = NOK
Lee Kesler method for petroleum fractions	DAT TC KE = LEE
Watson method for petroleum fraction	DAT TC KE = WAT
Critical pressure prediction method (select ONE of the following five options)	
Cavett method for petroleum fractions (default)	DAT PTC KE = CAV
Coal liquids method for petroleum fractions	DAT PC KE = COAL
Herzog method for saturated and unsaturated hydrocarbons	DAT PC KE = HERZ
Lee Kesler method for petroleum fractions	DAT PC KE = LEE
Watson method for petroleum fraction	DAT PC KE = WAT
Molecular weight prediction method (select ONE of the following four options)	
Cavett method (default option if petroleum fractions are entered GENERAL section)	DAT MOL KE = CAV
American Petroleum Institute method (should be avoided for light hydrocarbons)	DAT MOL KE = API
Hari method for petroleum fractions (default if CRUDE section present)	DAT MOL KE = HAR
Lee Kesler method for petroleum fractions	DAT MOL KE = LEE
Petroleum fractions heating values (select any of the following commands)	
High (wet heating value for petroleum fraction "i" where "i" is the component ID number)	HIG HEA (H units/molar Q units) i =
Low heating value for petroleum fraction "i", where "i" is the component ID number	LOW HEA (H units/molar Q units) i =
Desired carbon to hydrogen weight ratio for petroleum fraction "i", where "i" is the component ID number	CAR HYD i =
Peneloux correction to Soave Density	
This optional command is used to correct the density calculated using SOAVED. If not given for petroleum fractions default values of Paraffins=0.7, Naphthenes=0.2, Aromatics=0.1, and calculated carbon number will be used.	PNA FRA i = P vol.frac, N vol. frac, A vol. frac, carbon number

## Thermodynamics STEP 7

**Enter the commands listed below if the LOST work command is in the GENERAL section OR EQU REA module is present in the flowsheet.**

Additional component specification for COMPONENT ID numbers greater than 98	
Heat of formation for component "i", where "i" is the component ID number	HEA FOR (H units/molar Q units) i =
Heat of formation for component "i" for liquid phase, where "i" is the component ID number (required for PLUG flow REACTOR and CSTR when feed is a liquid and the ID number is >98)	HEA FOR LIQ (H units/molar Q units) i =
Entropy of formation for component "i", where "i" is the component ID number	ENT FOR (H units/molar Q units/T units) i =

## Thermodynamics: Notes

### Thermodynamics Quick Guide

#### Thermodynamics: Gas Processing and Petroleum Refining

OPTIONS K & Enthalpy	SYSTEM	TEMP. RANGE oF	PRES. RANGE PSIA	REMARKS
STDK STDH	Light HC's, H <sub>2</sub> , Gas Oil, Natural Gas (Water Immiscible)	0 to 930 Below Crit. Temp	14.7 to 3000	1. Do not use for a system with few mole% H <sub>2</sub> S, CO <sub>2</sub> 2. Do not use for close boiling Mixture (Xylene, Ethylene, Ethane sepn.)
APISOAVEK APISOAVEH	Light HC's and H <sub>2</sub> , H <sub>2</sub> S, CO <sub>2</sub> , CO, N <sub>2</sub>	0 to 990 Below Crit. Temp	14.7 to 4000	User's VLE data can be fitted to parameters via ChemTran.
SKDK SKDH	3-Phase H <sub>2</sub> O & HC's	0 to 990 Below Crit. Temp	14.7 to 2000	Requires multi-phase flash for rigorous 3 phase flash. Finds HC solubility in water phase.
BWRSK	Very accurate for HC's	0 to 930	Below 5000	

## Chapter 7

BWRSH	with CH4 to Undecane, Ethylene, Propylene, N2, CO2, H2S (Water Immiscible)				
KVALK APIMODH	High CH4 (N2 Rejection, Cryogenic Expander Plants)	-365 to 105	Below 6050		Enthalpy very accurate for light Hydrocarbons.
MODESSOK APIMODH	Heavy and Aromatic HC's (Water Immiscible)	50 to 1700	Below 75		Good for Vacuum Columns.
ESSOTABK APIMODH	Crude Oils (Water Immiscible)	65 to 930	Below 75		Improved enthalpy accuracy near Critical Region.
VAPPREK APIMODH	Crude Oils (Water Immiscible)	Known	Known		Used when calculation simplicity is required.

### **Thermodynamics: Petro-Chemical and Chemical Process**

<b>OPTIONS K &amp; Enthalpy</b>	<b>SYSTEM</b>	<b>TEMP. RANGE oF</b>	<b>PRES. RANGE PSIA</b>	<b>REMARKS</b>
RENK(NRTL) LATH	Non-ideal, Partially or Totally Miscible, e.g. Alcohol-Water, Acid-Water Ether - Alcohol, etc (USE CHEMTRAN TO REGRESS VLE/LLE DATA)	Known	Known	<ol style="list-style-type: none"> <li>1. User's VLE/LLE data Fitted to RENon parameters via ChemTran</li> <li>2. When VLE/LLE data not available calculate activity coefficients by UNIFAC and fit them to RENon parameters.</li> </ol>
WILK LATH	Non-ideal, Miscible Mixtures only. e.g. Alcohol-Water, Acid-Water (USE CHEMTRAN TO REGRESS VLE DATA)	Known	Known	<ol style="list-style-type: none"> <li>1. User's VLE data fitted to WILson parameters via ChemTran.</li> <li>2. When VLE data is not available calculate activity coefficients by UNIFAC and fit them to WILson parameters.</li> </ol>
UNIFACK LATH	Non-ideal Mixtures with Condensable Gases only. (no CH4, CO, CO2, N2, H2, etc..) Miscible Mixtures only.	86 to 260	1 to 3 ATM	<ol style="list-style-type: none"> <li>1. VLE only.</li> <li>2. Liquid Enthalpies from Latent Heat/ Component Database.</li> <li>3. Vapor Enthalpies from Redlich Kwong (STDK)</li> <li>4. No Liquid Heat of Mixing.</li> <li>5. Approximation Technique via Group Contribution.</li> </ol>
UNIQUEACK LATH	Non-ideal, Partially or Totally Miscible Mixtures (USE CHEMTRAN TO REGRESS VLE/LLE DATA)	Known	Known	<ol style="list-style-type: none"> <li>1. User's VLE/LLE data Fitted to UNIQUEAC parameters via ChemTran.</li> <li>2. When VLE/LLE data not available calculate activity coefficients by UNIFAC and fit them to UNIQUEAC parameters.</li> <li>3. Require R and Q parameters for Unknown Components.</li> </ol>
PENK PENH	Cryogenic C2H6/ C3H8 Recovery, HC mixture with high H2S & CO2, propane/propylene, C6H6/Toluene/ N2 Rejection. (Default, Water Immiscible)	0 to 990	14.7 to 6000	<ol style="list-style-type: none"> <li>1. Recommend usage of IMM=62 (immiscible water) &amp; ChemShare Binary Interaction Library (BINPAR=PENG1).</li> <li>2. User's VLE data can be fitted via ChemTran</li> <li>3. Accurate for Natural Gas Mixtures at Critical Region.</li> </ol>
LL UNIFACK LATH	Non-ideal Immiscible Mixtures	Known	Known	<ol style="list-style-type: none"> <li>1. LLE only, similar to UNIFACK.</li> <li>2. Approximation Technique</li> </ol>

### **Thermodynamics: Gas Treating Processes**



OPTIONS K & Enthalpy	SYSTEM	TEMP. RANGE oF	PRES. RANGE PSIA	REMARKS
APISOURK YENH	Water systems with H2S, CO2, NH3, N2 (Water Totally Miscible)	68 to 285	14.7 to 200	1. Acid Gas Concentration from 0 to 4 moles/kg of solution. 2. pH range from 2 to 14
SOURK YENH	Water systems with H2S, NH3. (Water Totally Miscible)	68 to 285	14.7 to 200	IF the NH3/H2S ratio exceeds the range of 1.5 to 20, APISOURK will be automatically used.
EPSOURK EPSOURH	Water systems with H2S, NH3, SO2, HCN, etc. (Water Totally Miscible)	68 to 285	14.7 to 200	Preferred over APISOURK and SOURK when all components are present from Henry's Constants in Water List.
MDEAK MDEAH	Removing CO2, H2S from Natural gas using Mono- or Di-ethanolamine (MEA, DEA)	68 to 285	14.7 to 1050	1. NOT for MDEA (only for MEA and DEA used separately) 2. NO Amine Blends are allowed (use "AMINEK" method) 3. Uses Equilibrium Approach only.
AMINEK AMINEH	Removing CO2, H2S from Sour Natural gas using MEA, DEA, MDEA, DGA, and DIPA	68 to 285	14.7 to 1050	1. Only for "Mixed Amine" for limited number of components. 2. Select same method for density and ALL transport properties. 3. Uses both Equilibrium and Rate- Based (Kinetic) approach for real tray simulation.
STEAM TABLES	PURE Water systems only	Known	Known	1. NBS/NRC Steam Tables for all properties. 2. When used with main Thermo options, pure water streams will use STEam TABLEs option.

**NOTE:** Various choices for DENSITY, VISCOSITY, & THERMAL CONDUCTIVITY (about 25 in all) correlations are available within DESIGN II. The user is recommended to choose the correlation that best represents their system of components and the range of temperature and pressure. Typically any DENSITY correlation determines pumping needs, line pressure drops, and tray hydraulic calculations. Please feel free to contact our Technical Support (support@winsim.com or 281-565-6700 x106) for further information.

## Thermodynamics Table 1. APISOAVEK Interaction Parameter List

To describe realistically the Gibbs energy, the ideal model is usually not sufficient and then there are many possibilities open for the choice of model. One choice is APISOAVE equation of state. In the regular model a parameter for each pair of constituents of the phase is introduced. This "binary interaction" parameter (BIP) can also be given some physical significance by comparing with the difference in bond energies between like and unlike atoms. The parameter is multiplied with the fractions of the two constituents and thus the parameter gives no contribution when any of the fractions is zero. And when the components do not have interactions including like component interactions, the parameters are assumed to be ideal and a value of one is used.

For most of the binary interactions within the DESIGN II database, the interaction parameters have been regressed from available data. However, they can be changed to fine tune the model ([Inline Fortran: Table 7. Thermodynamic Interaction Parameters](#)) to a particular point or set of data ([ChemTran: APISOAVE Parameters](#)). If additional data is available ([ChemTran: Database Sources for VLE and LLE Data](#)), it is possible to regress experimental VLE data via ChemTran ([ChemTran Correlating Mixture Data](#)).

The program stores default values of API Soave binary interaction parameters which were found by examining data for each available pair of components. In general, the model predictions and phase equilibrium tends to be very sensitive to the binary interaction parameters, so care should be taken in including and adjusting them. Details to set-up the DESIGN II simulation file to access the ChemTran generated data file can be found in [ChemTran File Access Commands](#).

**NOTES:** APISOAVE is usually used for mixtures of light gases and hydrocarbons in Natural Gas Processing. Please see [Thermodynamics Quick Guide](#). Also consider the Peng-Robinson and BWR, and BWRS equations of state..

## Chapter 7

DESIGN II ID	Component	H2S	CO2	N2	CO
50	H2S	-	X	X	-
49	CO2	X	-	-	X
46	N2	X	X	-	X
48	CO	-	X	X	-
2	methane	X	X	X	X
3	ethane	X	X	X	X
23	propylene	-	X	-	-
4	propane	X	X	X	X
5	i-butane	X	X	X	-
6	n-butane	X	X	X	-
7	i-pentane	-	X	-	-
8	n-pentane	X	X	-	-
10	hexane	-	-	X	-
11	heptane	X	X	-	-
12	octane	-	-	-	X
13	nonane	X	-	-	-
14	decane	X	X	X	-
38	cyclohexane	-	X	-	-
4172	iso-propylcyclohexane	X	-	-	X
40	benzene	-	X	X	-
7049	1,3,5 trimethylbenzene	X	-	-	-

### Thermodynamics Table 2. AGR Solvent (DMPEG) Absorption Modeling

The following components are available when AGR Solvent (DMPEG) absorption modeling is performed.

ID	Component	ID	Component	ID	Component
65	ACETYLENE	22	ETHYLENE	12	OCTANE
63	AMMONIA	11	HEPTANE	8	n-PENTANE
40	BENZENE	10	HEXANE	46	NITROGEN
6	n-BUTANE	1	HYDROGEN	4	PROPANE
49	CARBON DIOXIDE	1018	HYDROGEN CYANIDE	1024	THIOPHENE
1069	CARBON DISULFIDE	50	HYDROGEN SULFIDE	41	TOLUENE
48	CARBON MONOXIDE	5	ISO-BUTANE	2	METHANE
1087	CARBONYL SULFIDE	7	ISO-PENTANE	13	NONANE
14	DECANE	15	UNDECANE	62	WATER
1075	DICHLOROMETHANE	1059	METHYL MERCAPTAN	44	p-XYLENE
3	ETHANE	3058	PERCHLOROETHYLENE		
1012	ETHANOL	1140	TRICHLOROETHYLENE		

If you use other components, DESIGN II will use Chao-Seader K-values for those components. As the calculation technique and pure component property data for AGR Solvent-DMPEG are proprietary (AGR Solvent® is a registered trademark of Coastal Chemical Company.)

### Thermodynamics Table 3. Peng Robinson Binary Interaction Parameters

To describe realistically the Gibbs energy, the ideal model is usually not sufficient and then there are many possibilities open for the choice of model. One choice is Peng-Robinson equation of state (default.) In the regular model a parameter for each pair of constituents of the phase is introduced. This "binary interaction" parameter (BIP) can also be given some physical significance by comparing with the difference in bond energies between like and unlike atoms. The parameter is multiplied with the fractions of the two constituents and thus the parameter gives no contribution when any of the fractions is zero. And when the components do not have interactions including like component interactions, the parameters are assumed to be ideal and a value of one is used.

For most of the binary interactions within the DESIGN II database, the interaction parameters have been regressed from available data. However, they can be changed to fine tune the model ([Inline Fortran: Table 7. Thermodynamic Interaction Parameters](#)) to a particular point or set of data ([ChemTran: PENg Robinson Parameters](#)). If additional data is available ([ChemTran: Database Sources for VLE and LLE Data](#)), it is possible to regress experimental VLE data via ChemTran ([ChemTran Correlating Mixture Data](#)).

The program stores default values of Peng-Robinson binary interaction parameters which were found by examining data for each available pair of components (see notes below). In general, the model predictions and phase equilibrium tends to be

very sensitive to the binary interaction parameters, so care should be taken to choose the best available literature equilibrium data that closely represent the process conditions. Details to set-up the DESIGN II simulation file to access the ChemTran generated data file can be found in [ChemTran File Access Commands](#).

## NOTES:

1. Peng-Robinson is usually used for mixtures of light gases and hydrocarbons in Natural Gas Processing. Please see [Thermodynamics Quick Guide](#). Also consider the APISOAVE and BWR, and BWRS equations of state.
2. The stored Peng-Robinson parameter library database is used via the command **BIN PAR = PENG1**. In flowsheets created with DESIGN II for Windows Versions 8.26 or up, it is automatically activated when Peng-Robinson K-value method is chosen under basic thermodynamics. For earlier Versions, the command can be activated by the user via Specify...Advanced Thermo in the flowsheet or by adding the command in the GENERAL section of the input file.
3. Peng-Robinson data library file for petroleum fractions requires activation of the command **PET BIN PAR = GPA1**. This can be optionally activated by the user via Specify...Advanced Thermo in the flowsheet or by adding the command in the GENERAL section of the input file.

Component ID Number	Name of 1st Component	Component ID Number	Name of 2nd Component
1002	ACETONE	3	ETHANE
65	ACETYLENE	22	ETHYLENE
63	AMMONIA	1171	ARGON
63	AMMONIA	46	NITROGEN
63	AMMONIA	62	WATER
3004	AMYL ALCOHOL	54	2,2-DIMETHYLBUTANE
3004	AMYL ALCOHOL	55	2,3-DIMETHYLBUTANE
3004	AMYL ALCOHOL	10	n-HEXANE
3004	AMYL ALCOHOL	52	2-METHYLPENTANE
3004	AMYL ALCOHOL	53	3-METHYLPENTANE
1171	ARGON	63	AMMONIA
1171	ARGON	2	METHANE
1171	ARGON	46	NITROGEN
1171	ARGON	47	OXYGEN
40	BENZENE	49	CARBON DIOXIDE
40	BENZENE	3	ETHANE
40	BENZENE	22	ETHYLENE
40	BENZENE	11	n-HEPTANE
40	BENZENE	5002	HEXAFLUOROBENZENE
40	BENZENE	10	n-HEXANE
40	BENZENE	2	METHANE
40	BENZENE	12	n-OCTANE
40	BENZENE	8	n-PENTANE
40	BENZENE	4	PROPANE
28	1,3-BUTADIENE	6	n-BUTANE
28	1,3-BUTADIENE	24	1-BUTENE
6	n-BUTANE	28	1,3-BUTADIENE
6	n-BUTANE	24	1-BUTENE
6	n-BUTANE	49	CARBON DIOXIDE
6	n-BUTANE	14	n-DECANE
6	n-BUTANE	3	ETHANE
6	n-BUTANE	22	ETHYLENE
6	n-BUTANE	11	n-HEPTANE
6	n-BUTANE	10	n-HEXANE
6	n-BUTANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
6	n-BUTANE	1	HYDROGEN
6	n-BUTANE	5	i-BUTANE
6	n-BUTANE	2	METHANE
6	n-BUTANE	46	NITROGEN
6	n-BUTANE	8	n-PENTANE
6	n-BUTANE	4	PROPANE
24	1-BUTENE	28	1,3-BUTADIENE
24	1-BUTENE	6	n-BUTANE
24	1-BUTENE	49	CARBON DIOXIDE
24	1-BUTENE	23	PROPYLENE
49	CARBON DIOXIDE	40	BENZENE
49	CARBON DIOXIDE	6	n-BUTANE
49	CARBON DIOXIDE	24	1-BUTENE
49	CARBON DIOXIDE	38	CYCLOHEXANE
49	CARBON DIOXIDE	14	n-DECANE
49	CARBON DIOXIDE	1176	DICHLORODIFLUOROMETHANE

## Chapter 7

49	CARBON DIOXIDE	1005	DIETHYL ETHER
49	CARBON DIOXIDE	3047	DIFLUOROMETHANE
49	CARBON DIOXIDE	3	ETHANE
49	CARBON DIOXIDE	22	ETHYLENE
49	CARBON DIOXIDE	11	n-HEPTANE
49	CARBON DIOXIDE	10	n-HEXANE
49	CARBON DIOXIDE	1,1000	HYDROGEN, HYDROGEN (PARA)
49	CARBON DIOXIDE	1	HYDROGEN
49	CARBON DIOXIDE	50	HYDROGEN SULFIDE
49	CARBON DIOXIDE	5	i-BUTANE
49	CARBON DIOXIDE	7	ISOPENTANE
49	CARBON DIOXIDE	2	METHANE
49	CARBON DIOXIDE	1021	METHANOL
49	CARBON DIOXIDE	2003	METHYL ACETATE
49	CARBON DIOXIDE	46	NITROGEN
49	CARBON DIOXIDE	1043	NITROUS OXIDE
49	CARBON DIOXIDE	8	n-PENTANE
49	CARBON DIOXIDE	4	PROPANE
49	CARBON DIOXIDE	23	PROPYLENE
49	CARBON DIOXIDE	41	TOLUENE
49	CARBON DIOXIDE	62	WATER
49	CARBON DIOXIDE	3103	ETHYLENE GLYCOL (MEG OR EG)
49	CARBON DIOXIDE	4030	DI-ETHYLENE GLYCOL (DEG)
49	CARBON DIOXIDE	4044	TRI-ETHYLENE GLYCOL (TEG)
48	CARBON MONOXIDE	3	ETHANE
48	CARBON MONOXIDE	1,1000	HYDROGEN, HYDROGEN (PARA)
48	CARBON MONOXIDE	50	HYDROGEN SULFIDE
48	CARBON MONOXIDE	2	METHANE
48	CARBON MONOXIDE	46	NITROGEN
48	CARBON MONOXIDE	4	PROPANE
1052	CARBON TETRAFLUORIDE	1114	TRIFLUOROMETHANE
1087	CARBONYL SULFIDE	2	METHANE
1087	CARBONYL SULFIDE	4	PROPANE
1154	CHLORODIFLUOROMETHANE	1122	CHLOROPENTAFLUOROETHANE
1154	CHLORODIFLUOROMETHANE	1176	DICHLORODIFLUOROMETHANE
1122	CHLOROPENTAFLUOROETHANE	1154	CHLORODIFLUOROMETHANE
1155	CHLOROTRIFLUOROMETHANE	1176	DICHLORODIFLUOROMETHANE
115	CHLOROTRIFLUOROMETHANE	1114	TRIFLUOROMETHANE
1036	m-CRESOL	2	METHANE
38	CYCLOHEXANE	49	CARBON DIOXIDE
38	CYCLOHEXANE	1072	CYCLOHEXANONE
38	CYCLOHEXANE	7043	CYCLOHEXENE
38	CYCLOHEXANE	1028	1,2-DICHLOROETHANE
38	CYCLOHEXANE	3	ETHANE
38	CYCLOHEXANE	10	n-HEXANE
38	CYCLOHEXANE	2	METHANE
38	CYCLOHEXANE	8	n-PENTANE
1072	CYCLOHEXANONE	38	CYCLOHEXANE
7043	CYCLOHEXENE	38	CYCLOHEXANE
7043	CYCLOHEXENE	1028	1,2-DICHLOROETHANE
14	n-DECANE	6	n-BUTANE
14	n-DECANE	49	CARBON DIOXIDE
14	n-DECANE	3	ETHANE
14	n-DECANE	2	METHANE
1176	DICHLORODIFLUOROMETHANE	49	CARBON DIOXIDE
1176	DICHLORODIFLUOROMETHANE	1154	CHLORODIFLUOROMETHANE
1176	DICHLORODIFLUOROMETHANE	1155	CHLOROTRIFLUOROMETHANE
1176	DICHLORODIFLUOROMETHANE	46	NITROGEN
1028	1,2-DICHLOROETHANE	38	CYCLOHEXANE
1028	1,2-DICHLOROETHANE	7043	CYCLOHEXENE
1005	DIETHYL ETHER	49	CARBON DIOXIDE
1005	DIETHYL ETHER	3	ETHANE
3047	DIFLUOROMETHANE	49	CARBON DIOXIDE
54	2,2-DIMETHYLBUTANE	3004	AMYL ALCOHOL
55	2,3-DIMETHYLBUTANE	3004	AMYL ALCOHOL
4178	DIPHENYLMETHANE	2	METHANE
3	ETHANE	1002	ACETONE
3	ETHANE	40	BENZENE
3	ETHANE	6	n-BUTANE
3	ETHANE	49	CARBON DIOXIDE
3	ETHANE	48	CARBON MONOXIDE
3	ETHANE	38	CYCLOHEXANE
3	ETHANE	14	n-DECANE
3	ETHANE	1005	DIETHYL ETHER
3	ETHANE	22	ETHYLENE
3	ETHANE	11	n-HEPTANE
3	ETHANE	10	n-HEXANE

3	ETHANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
3	ETHANE	50	HYDROGEN SULFIDE
3	ETHANE	5	i-BUTANE
3	ETHANE	2	METHANE
3	ETHANE	1021	METHANOL
3	ETHANE	2003	METHYL ACETATE
3	ETHANE	46	NITROGEN
3	ETHANE	12	n-OCTANE
3	ETHANE	8	n-PENTANE
3	ETHANE	4	PROPANE
3	ETHANE	23	PROPYLENE
3	ETHANE	3103	ETHYLENE GLYCOL (MEG OR EG)
3	ETHANE	4030	DI-ETHYLENE GLYCOL (DEG)
3	ETHANE	4044	TRI-ETHYLENE GLYCOL (TEG)
1012	ETHANOL	4	PROPANE
22	ETHYLENE	65	ACETYLENE
22	ETHYLENE	40	BENZENE
22	ETHYLENE	6	n-BUTANE
22	ETHYLENE	49	CARBON DIOXIDE
22	ETHYLENE	3	ETHANE
22	ETHYLENE	11	n-HEPTANE
22	ETHYLENE	1, 1000	HYDROGEN, HYDROGEN (PARA)
22	ETHYLENE	2	METHANE
22	ETHYLENE	46	NITROGEN
1172	HELIUM	11	n-HEPTANE
1172	HELIUM	2	METHANE
1172	HELIUM	46	NITROGEN
1172	HELIUM	4	PROPANE
11	n-HEPTANE	40	BENZENE
11	n-HEPTANE	6	n-BUTANE
11	n-HEPTANE	49	CARBON DIOXIDE
11	n-HEPTANE	3	ETHANE
11	n-HEPTANE	22	ETHYLENE
11	n-HEPTANE	1172	HELIUM
11	n-HEPTANE	10	n-HEXANE
11	n-HEPTANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
11	n-HEPTANE	2	METHANE
11	n-HEPTANE	8	n-PENTANE
11	n-HEPTANE	1049	2-PENTANONE
11	n-HEPTANE	4	PROPANE
5002	HEXAFLUOROBENZENE	40	BENZENE
5002	HEXAFLUOROBENZENE	10	n-HEXANE
5002	HEXAFLUOROBENZENE	39	METHYLCYCLOHEXANE
5002	HEXAFLUOROBENZENE	41	TOLUENE
10	n-HEXANE	3004	AMYL ALCOHOL
10	n-HEXANE	40	BENZENE
10	n-HEXANE	6	n-BUTANE
10	n-HEXANE	49	CARBON DIOXIDE
10	n-HEXANE	38	CYCLOHEXANE
10	n-HEXANE	3	ETHANE
10	n-HEXANE	11	n-HEPTANE
10	n-HEXANE	5002	HEXAFLUOROBENZENE
10	n-HEXANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
10	n-HEXANE	1019	ISOPROPANOL
10	n-HEXANE	2	METHANE
10	n-HEXANE	46	NITROGEN
10	n-HEXANE	4	PROPANE
10	n-HEXANE	3005	TERT-AMYL ALCOHOL
1, 1000	HYDROGEN, HYDROGEN (PARA)	6	n-BUTANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	49	CARBON DIOXIDE
1, 1000	HYDROGEN, HYDROGEN (PARA)	48	CARBON MONOXIDE
1, 1000	HYDROGEN, HYDROGEN (PARA)	3	ETHANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	22	ETHYLENE
1, 1000	HYDROGEN, HYDROGEN (PARA)	11	n-HEPTANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	10	n-HEXANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	2	METHANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	3175	1-METHYLNAPHTHALENE
1, 1000	HYDROGEN, HYDROGEN (PARA)	46	NITROGEN
1, 1000	HYDROGEN, HYDROGEN (PARA)	4	PROPANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	23	PROPYLENE
1, 1000	HYDROGEN, HYDROGEN (PARA)	4028	QUINOLINE
1, 1000	HYDROGEN, HYDROGEN (PARA)	3147	TETRALIN
1, 1000	HYDROGEN, HYDROGEN (PARA)	41	TOLUENE
50	HYDROGEN SULFIDE	49	CARBON DIOXIDE
50	HYDROGEN SULFIDE	48	CARBON MONOXIDE
50	HYDROGEN SULFIDE	3	ETHANE
50	HYDROGEN SULFIDE	5	i-BUTANE

# Chapter 7

50	HYDROGEN SULFIDE	46	NITROGEN
50	HYDROGEN SULFIDE	62	WATER
5	i-BUTANE	6	n-BUTANE
5	i-BUTANE	49	CARBON DIOXIDE
5	i-BUTANE	3	ETHANE
5	i-BUTANE	50	HYDROGEN SULFIDE
5	i-BUTANE	2	METHANE
5	i-BUTANE	46	NITROGEN
5	i-BUTANE	4	PROPANE
5	i-BUTANE	23	PROPYLENE
7	ISOPENTANE	49	CARBON DIOXIDE
7	ISOPENTANE	2	METHANE
7	ISOPENTANE	46	NITROGEN
7	ISOPENTANE	8	n-PENTANE
7	ISOPENTANE	4	PROPANE
1019	ISOPROPANOL	10	n-HEXANE
1174	KRYPTON	47	OXYGEN
2	METHANE	1171	ARGON
2	METHANE	40	BENZENE
2	METHANE	6	n-BUTANE
2	METHANE	49	CARBON DIOXIDE
2	METHANE	48	CARBON MONOXIDE
2	METHANE	1087	CARBONYL SULFIDE
2	METHANE	1036	m-CRESOL
2	METHANE	38	CYCLOHEXANE
2	METHANE	14	n-DECANE
2	METHANE	4178	DIPHENYLMETHANE
2	METHANE	3	ETHANE
2	METHANE	22	ETHYLENE
2	METHANE	1172	HELIUM
2	METHANE	11	n-HEPTANE
2	METHANE	10	n-HEXANE
2	METHANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
2	METHANE	5	i-BUTANE
2	METHANE	7	ISOPENTANE
2	METHANE	3175	1-METHYLNAPHTHALENE
2	METHANE	46	NITROGEN
2	METHANE	1043	NITROUS OXIDE
2	METHANE	13	n-NONANE
2	METHANE	12	n-OCTANE
2	METHANE	8	n-PENTANE
2	METHANE	4	PROPANE
2	METHANE	3147	TETRALIN
2	METHANE	41	TOLUENE
2	METHANE	43	m-XYLENE
2	METHANE	3103	ETHYLENE GLYCOL (MEG OR EG)
2	METHANE	4030	DI-ETHYLENE GLYCOL (DEG)
2	METHANE	4044	TRI-ETHYLENE GLYCOL (TEG)
1021	METHANOL	49	CARBON DIOXIDE
1021	METHANOL	2	METHANE
1021	METHANOL	3	ETHANE
1021	METHANOL	46	NITROGEN
1021	METHANOL	62	WATER
2003	METHYL ACETATE	49	CARBON DIOXIDE
2003	METHYL ACETATE	3	ETHANE
39	METHYLCYCLOHEXANE	5002	HEXAFLUOROBENZENE
3175	1-METHYLNAPHTHALENE	1, 1000	HYDROGEN, HYDROGEN (PARA)
3175	1-METHYLNAPHTHALENE	2	METHANE
52	2-METHYLPENTANE	3004	AMYL ALCOHOL
53	3-METHYLPENTANE	3004	AMYL ALCOHOL
46	NITROGEN	63	AMMONIA
46	NITROGEN	1171	ARGON
46	NITROGEN	6	n-BUTANE
46	NITROGEN	49	CARBON DIOXIDE
46	NITROGEN	48	CARBON MONOXIDE
46	NITROGEN	1176	DICHLORODIFLUOROMETHANE
46	NITROGEN	3	ETHANE
46	NITROGEN	22	ETHYLENE
46	NITROGEN	1172	HELIUM
46	NITROGEN	10	n-HEXANE
46	NITROGEN	1, 1000	HYDROGEN, HYDROGEN (PARA)
46	NITROGEN	50	HYDROGEN SULFIDE
46	NITROGEN	5	i-BUTANE
46	NITROGEN	7	ISOPENTANE
46	NITROGEN	2	METHANE
46	NITROGEN	1021	METHANOL
46	NITROGEN	1043	NITROUS OXIDE

46	NITROGEN	47	OXYGEN
46	NITROGEN	8	n-PENTANE
46	NITROGEN	4	PROPANE
46	NITROGEN	23	PROPYLENE
46	NITROGEN	3103	ETHYLENE GLYCOL (MEG OR EG)
1043	NITROUS OXIDE	49	CARBON DIOXIDE
1043	NITROUS OXIDE	2	METHANE
1043	NITROUS OXIDE	46	NITROGEN
1043	NITROUS OXIDE	47	OXYGEN
13	n-NONANE	2	METHANE
12	n-OCTANE	40	BENZENE
12	n-OCTANE	3	ETHANE
12	n-OCTANE	2	METHANE
47	OXYGEN	1171	ARGON
47	OXYGEN	1174	KRYPTON
47	OXYGEN	46	NITROGEN
47	OXYGEN	1043	NITROUS OXIDE
8	n-PENTANE	40	BENZENE
8	n-PENTANE	6	n-BUTANE
8	n-PENTANE	49	CARBON DIOXIDE
8	n-PENTANE	38	CYCLOHEXANE
8	n-PENTANE	3	ETHANE
8	n-PENTANE	11	n-HEPTANE
8	n-PENTANE	7	ISOPENTANE
8	n-PENTANE	2	METHANE
8	n-PENTANE	46	NITROGEN
8	n-PENTANE	4	PROPANE
1049	2-PENTANONE	11	n-HEPTANE
4	PROPANE	40	BENZENE
4	PROPANE	6	n-BUTANE
4	PROPANE	49	CARBON DIOXIDE
4	PROPANE	48	CARBON MONOXIDE
4	PROPANE	1087	CARBONYL SULFIDE
4	PROPANE	3	ETHANE
4	PROPANE	1012	ETHANOL
4	PROPANE	1172	HELIUM
4	PROPANE	11	n-HEPTANE
4	PROPANE	10	n-HEXANE
4	PROPANE	1, 1000	HYDROGEN, HYDROGEN (PARA)
4	PROPANE	5	i-BUTANE
4	PROPANE	7	ISOPENTANE
4	PROPANE	2	METHANE
4	PROPANE	46	NITROGEN
4	PROPANE	8	n-PENTANE
4	PROPANE	23	PROPYLENE
4	PROPANE	4044	TRI-ETHYLENE GLYCOL (TEG)
23	PROPYLENE	24	1-BUTENE
23	PROPYLENE	49	CARBON DIOXIDE
23	PROPYLENE	3	ETHANE
23	PROPYLENE	1, 1000	HYDROGEN, HYDROGEN (PARA)
23	PROPYLENE	5	i-BUTANE
23	PROPYLENE	46	NITROGEN
23	PROPYLENE	4	PROPANE
4028	QUINOLINE	1, 1000	HYDROGEN, HYDROGEN (PARA)
3005	TERT-AMYL ALCOHOL	10	n-HEXANE
3051	1,1,2,2-TETRACHLOROETHANE	41	TOLUENE
3147	TETRALIN	1	HYDROGEN
3147	TETRALIN	2	METHANE
41	TOLUENE	49	CARBON DIOXIDE
41	TOLUENE	5002	HEXAFLUOROBENZENE
41	TOLUENE	1, 1000	HYDROGEN, HYDROGEN (PARA)
41	TOLUENE	2	METHANE
41	TOLUENE	3051	1,1,2,2-TETRACHLOROETHANE
1114	TRIFLUOROMETHANE	1052	CARBON TETRAFLUORIDE
1114	TRIFLUOROMETHANE	1155	CHLOROTRIFLUOROMETHANE
62	WATER	63	AMMONIA
62	WATER	49	CARBON DIOXIDE
62	WATER	50	HYDROGEN SULFIDE
62	WATER	1021	METHANOL
43	m-XYLENE	2	METHANE

**Thermodynamics Table 4. Lee- Kesler Binary Interaction Parameters**

To describe realistically the Gibbs energy, the ideal model is usually not sufficient and then there are many possibilities open for the choice of model. One choice is Peng-Robinson equation of state (default). In the regular model a parameter for each

## Chapter 7

pair of constituents of the phase is introduced. This "binary interaction" parameter (BIP) can also be given some physical significance by comparing with the difference in bond energies between like and unlike atoms. The parameter is multiplied with the fractions of the two constituents and thus the parameter gives no contribution when any of the fractions is zero. And when the components do not have interactions including like component interactions, the parameters are assumed to be ideal and a value of one is used.

For most of the binary interactions within the DESIGN II database, the interaction parameters have been regressed from available data. At this time, Lee-Kesler correlation is not enabled in ChemTran for addition via data regression or in Inline Fortran for adjusting them.

The program stores default values of Lee-Kesler binary interaction parameters which were found by examining data for each available pair of components. In general, the model predictions and phase equilibrium tends to be very sensitive to the binary interaction parameters, so care should be taken in including and adjusting them.

Component ID Number	Name of 1st Component	Component ID Number	Name of 2nd Component
65	ACETYLENE	22	ETHYLENE
63	AMMONIA	1171	ARGON
		46	NITROGEN
		62	WATER
1171	ARGON	63	AMMONIA
		2	METHANE
		46	NITROGEN
		47	OXYGEN
40	BENZENE	6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		82	i-OCTANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
28	1,3-BUTADIENE	6	n-BUTANE
		24	1-BUTENE
5	i-BUTANE	6	n-BUTANE
		49	CARBON DIOXIDE
		3	ETHANE
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		4	PROPANE
		23	PROPYLENE
6	n-BUTANE	40	BENZENE
		28	1,3-BUTADIENE
		5	i-BUTANE
		27	1-BUTENE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
27	i-BUTENE	28	1,3-BUTADIENE
		49	CARBON DIOXIDE
		23	PROPYLENE
49	CARBON DIOXIDE	40	BENZENE
		5	i-BUTANE



		6	n-BUTANE
		27	1-BUTENE
		38	CYCLOHEXANE
		14	n-DECANE
		3047	DIFLUOROMETHANE
		3	ETHANE
		1005	ETHYL ETHER
		1176	FREON12
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		1021	METHANOL
		39	METHYLCYCLOHEXANE
		46	NITROGEN
		1043	NITROUS OXIDE
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		41	TOLUENE
		62	WATER
		43	m-XYLENE
48	CARBON MONOXIDE	3	ETHANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
1036	m-CRESOL	2	METHANE
1122	CHLOROPENTAFLUOROETHANE	1154	FREON 22
1155	CHLOROTRIFLUOROMETHANE	1114	FLUOROFORM
		1176	DICHLORODIFLUOROMETHANE
38	CYCLOHEXANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		7043	CYCLOHEXENE
		14	n-DECANE
		1028	1,2-DICHLOROETHANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
7043	CYCLOHEXENE	38	CYCLOHEXANE
		1028	1,2-DICHLOROETHANE
14	DECANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
1176	DICHLORODIFLUOROMETHANE	1154	CHLORODIFLUOROMETHANE
		1155	CHLOROTRIFLUOROMETHANE
		46	NITROGEN
1028	1,2-DICHLOROETHANE	38	CYCLOHEXANE
		7043	CYCLOHEXENE
3047	DIFLUOROMETHANE	49	CARBON DIOXIDE
54	2,2-DIMETHYLBUTANE	3004	1-PENTANOL
55	2,3-DIMETHYLBUTANE	3004	1-PENTANOL
4178	DIPHENYLMETHANE	2	METHANE
3	ETHANE	40	BENZENE
		5	i-BUTANE
		6	n-BUTANE

		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		1021	METHANOL
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
1012	ETHANOL	4	PROPANE
22	ETHYLENE	65	ACETYLENE
		40	BENZENE
		6	n-BUTANE
		3	ETHANE
		11	n-HEPTANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
		46	NITROGEN
1005	ETHYL ETHER	49	CARBON DIOXIDE
1114	FLUOROFORM	1155	DICHLORODIFLUOROMETHANE
		1052	CHLOROPENTAFLUOROETHANE
1176	FREON12	49	CARBON DIOXIDE
1154	FREON 22	1176	DICHLORODIFLUOROMETHANE
		1122	CHLOROPENTAFLUOROETHANE
11	n-HEPTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		82	i-OCTANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
		10	n-HEXANE
		40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		3004	1-PENTANOL
		3005	t-PENTANOL
		4	PROPANE
1, 1000	HYDROGEN, HYDROGEN (PARA)	6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		3175	METHYL NAPHTHALENE
		46	NITROGEN

		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		3147	TETRALIN
		41	TOLUENE
50	HYDROGEN SULFIDE	5	i-BUTANE
		49	CARBON DIOXIDE
		14	n-DECANE
		11	n-HEPTANE
		39	METHYLCYCLOHEXANE
		46	NITROGEN
		8	n-PENTANE
		41	TOLUENE
1174	KRYPTON	43	m-XYLENE
2	METHANE	47	OXYGEN
		1171	ARGON
		40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		1036	m-CRESOL
		38	CYCLOHEXANE
		14	n-DECANE
		4178	DIPHENYLMETHANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		3175	1-METHYL NAPHTALENE
		46	NITROGEN
		1043	NITROUS OXIDE
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		3147	TETRALIN
		41	TOLUENE
		43	m-XYLENE
1021	METHANOL	49	CARBON DIOXIDE
		3	ETHANE
		62	WATER
39	METHYLCYCLOHEXANE	49	CARBON DIOXIDE
		50	HYDROGEN SULFIDE
3175	1-METHYL NAPHTHALENE	1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
52	2-METHYLPENTANE	3004	1-PENTANOL
53	3-METHYLPENTANE	3004	1-PENTANOL
46	NITROGEN	63	AMMONIA
		1171	ARGON
		40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		1176	FREON 12
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		1043	NITROUS OXIDE
		47	OXYGEN
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
1043	NITROUS OXIDE	49	CARBON DIOXIDE
		2	METHANE
		46	NITROGEN
		47	OXYGEN

# Chapter 7

13	n-NONANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		12	n-OCTANE
		8	n-PENTANE
82	i-OCTANE	4	PROPANE
		40	BENZENE
		11	n-HEPTANE
12	n-OCTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		13	n-NONANE
		8	n-PENTANE
		4	PROPANE
47	OXYGEN	1171	ARGON
		1174	KRYPTON
		46	NITROGEN
		1043	NITROUS OXIDE
7	i-PENTANE	6	n-BUTANE
		49	CARBON DIOXIDE
		3	ETHANE
		2	METHANE
		46	NITROGEN
		8	n-PENTANE
		4	PROPANE
8	n-PENTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		4	PROPANE
3004	1-PENTANOL	10	n-HEXANE
		54	2,2-DIMETHYLBUTANE
		55	2,3-DIMETHYLBUTANE
		52	2-METHYLPENTANE
		53	3-METHYLPENTANE
3005	t-PENTANOL	10	n-HEXANE
4	PROPANE	40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		1012	ETHANOL
		11	n-HEPTANE
		10	n-HEXANE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		23	PROPYLENE

1019	2-PROPANOL	10	n-HEXANE
23	PROPYLENE	5	i-BUTANE
		6	n-BUTANE
		27	i-BUTENE
		49	CARBON DIOXIDE
		3	ETHANE
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		4	PROPANE
3058	TETRACHLOROETHANE	41	TOLUENE
1052	TETRAFLUOROMETHENE	1114	FLUOROFORM
3147	TETRALIN	1, 1000	HYDROGEN, HYDROGEN (PARA)
		2	METHANE
41	TOLUENE	49	CARBON DIOXIDE
		1, 1000	HYDROGEN, HYDROGEN (PARA)
		50	HYDROGEN SULFIDE
		2	METHANE
		3058	TETRACHLOROETHENE
62	WATER	63	AMMONIA
		49	CARBON DIOXIDE
		1021	METHANOL
43	m-XYLENE	49	CARBON DIOXIDE
		50	HYDROGEN SULFIDE
		2	METHANE

## Thermodynamics Table 5. Henry's Constants in Water List

Henry's constants in water for the following components are built into the Pure Component Database. The source for these Henry's constants is Reference 19f, except for those components marked with (\*). Values for those components have been taken from Edwards, et al, Reference 19b.

I.D.	Name	I.D.	Name
1	Hydrogen	1014	Ethylamine
2	Methane	1018	Hydrogen cyanide (*)
3	Ethane	1037	Methyl chloride
4	Propane	1039	Fluoromethane
5	i-Butane	1041	Nitric oxide
6	n-Butane	1043	Nitrous oxide
22	Ethylene	1052	Carbon tetrafluoride
23	Propylene	1062	Chlorine
24	1-Butene (**)	1077	Methyl amine
27	i-Butene	1081	Dimethyl amine
28	1,3-Butadiene	1087	Carbonyl sulfide
46	Nitrogen	1125	Bromomethane
47	Oxygen	1137	Vinyl chloride
48	Carbon monoxide	1154	Freon 11
49	Carbon dioxide(*)	1156	Cyclopropane
50	Hydrogen sulfide(*)	1171	Argon
51	Sulfur dioxide(*)	1172	Helium
63	Ammonia (*)	1173	Neon
65	Acetylene	7048	Vinylacetylene
66	Propyne		
67	1-Butyne		
68	2-Methylpropene		

(\*\*) cis- and trans-2-Butene which are available for the MDEAK option are not in this library.

## Thermodynamics Table 6. Mixed Amine Modeling

The following components are the ONLY ones supported for the simulation of Mixed Amine model. Listed below are 47 components grouped for use along with the Amines (MEA, DEA, MDEA, DGA, and DIPA). Note that "Mixed Amine" method applies only to this set of components. If other components NOT in this list are present "Mixed Amine" thermodynamic approach will not be used.

Components available in Mixed Amine thermodynamics also form a subset of the components listed in Reid, Prausnitz and Sherwood's "The Properties of Gases and Liquids", Third Edition, McGraw-Hill Book Co, NY, 1977.

DESIGN II ID#	COMPONENT NAME	FORMULA
1	HYDROGEN	H2
2	METHANE	CH4
3	ETHANE	C2H6

## Chapter 7

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4	PROPANE	C3H8
5	ISOBUTANE; 2-METHYLPROPANE	C4H10
6	N-BUTANE	C4H10
7	ISOPENTANE	C5H12
8	N-PENTANE	C5H12
9	NEOPENTANE; 2,2-DIMETHYLPROPANE	C5H12
10	N-HEXANE	C6H14
11	N-HEPTANE	C7H16
22	ETHYLENE	C2H4
23	PROPYLENE; PROPENE	C3H6
24	1-BUTENE	C4H8
27	ISOBUTYLENE; 2-METHYLPROPENE	C4H8
28	1,3-BUTADIENE	C4H6
36	CYCLOPENTANE	C5H10
37	METHYLCYCLOPENTANE	C6H12
38	CYCLOHEXANE	C6H12
39	METHYL CYCLOHEXANE	C7H14
40	BENZENE	C6H6
41	TOLUENE	C7H8
42	o-XYLENE	C8H10
43	m-XYLENE	C8H10
44	p-XYLENE	C8H10
45	ETHYL BENZENE	C8H10
46	NITROGEN	N2
47	OXYGEN	O2
48	CARBON MONOXIDE	CO
49	CARBON DIOXIDE	CO2
50	HYDROGEN SULFIDE	H2S
62	WATER	H2O
65	ACETYLENE	C2H2
66	METHYLACETYLENE; PROPYNE	C3H4
67	ETHYLACETYLENE; 1-BUTYNE	C4H6
1087	CARBONYL SULFIDE	COS
1156	CYCLOPROPANE; TRIMETHYLENE	C3H6
1159	ISOHEXANE; 2-METHYL PENTANE	C6H14
1171	ARGON	AR
1172	HELIUM	HE
1219	PIPERAZINE	C4H10N2
2053	DIGLYCOLAMINE; DGA	C4H11NO2
4051	DIETHANOLAMINE; DEA	C4H11NO2
4155	MONOETHANOLAMINE; MEA	C2H7NO

6012	DIISOPROPANOLAMINE; DIPA	C6H15NO2
7048	VINYLCETYLENE; 1-BUTEN-3-YNE	C4H4
7051	METHYLDIETHANOLAMINE; MDEA	C5H13NO2

The key factor limiting the number of components is the lack of solubility data in water and the phase equilibria data on other pairs of system components.

Enter components into the components list and reference within DESIGN II by using either the component number or the component identifier.

**NOTE:**

1. Use of ChemTran is also not allowed when "Mixed Amine" thermodynamic method is selected.
2. The Henry's constants from neo-pentane are being used for 5 new components such as iso-pentane, n-pentane, n-hexane, n-heptane, and iso-hexane.

**Source:** GPSA Engineering Data Book, Chapter 21 – Eleventh Edition 1998, Aqueous Alkanolamine Processes (1)

	MEA	DEA	SNPA-DEA	DGA	SUFINOL	MDEA
Acid gas pickup, scf/gal @ 100°F, normal range (2)	3.1-4.3	3.8-5.0	6.7-8	4.7-6.6	4.0-17.0	3-7.5
Acid gas pickup, mols/mol amine, normal range (3)	0.33-0.40	0.35-0.65	0.72-1.02	0.25-0.3	NA	0.2-0.55
Lean solution residual acid gas, mol/mol amine, normal range (4)	0.12 ±	0.08 ±	0.08 ±	0.10 ±	NA	0.005-0.01
Rich solution acid gas loading, mol/mol amine, normal range (3)	0.45-0.52	0.43-0.73	0.8-1.1	0.35-0.40	NA	0.4-0.55
Solution concentration, wt%, normal range	15-25	25-35	25-30	50-70	3 comp varies	40-50
Approximate reboiler heat duty, Btu/gal lean solution (5)	1,000-1,200	900-1,000	900-1,000	1,100-1,300	350-750	800-1200
Steam heated reboiler tube bundle, approx. average heat flux, Q/A = MBtu/hr-ft <sup>2</sup> (6)	9-10	9-10	9-10	9-10	9-10	9-10
Direct fired reboiler fire tube, Average heat flux, Q/A = MBtu/hr-ft <sup>2</sup> (6)	8-10	8-10	8-10	8-10	8-10	8-10
Reclaimer, steam bundle or fire tube, Average heat flux, Q/A = MBtu/hr-ft <sup>2</sup> (6)	6-9	NA (7)	NA (7)	6-8	NA	NA
Reboiler temperature, normal Operating range, °F (8)	225-260	230-250	230-250	250-260	230-280	230-260
Heats of reaction; (10) approximate: Btu/lb H <sub>2</sub> S	550-670 (10)	500-600 (11)	511	674	NA	450-520
Btu/lb CO <sub>2</sub>	620-700	580-650	653	850	NA	570-600

NA — not applicable or not available

**NOTES:**

1. These data alone should not be used for specific design purposes. Many design factors must be considered for actual plant design.
2. Dependent upon acid gas partial pressures and solution concentrations.
3. Dependent upon acid gas partial pressures and corrosiveness of solution. Might be only 60% or less of value shown for corrosive systems.
4. Varies with stripper overhead reflux ratio. Low residual acid gas contents require more stripper trays and/or higher reflux ratios yielding larger reboiler duties.
5. Varies with stripper overhead reflux ratios, rich solution feed temperature to stripper and reboiler temperature.
6. Maximum A1point heat flux can reach 20,000-25,000 Btu/hr-ft<sup>2</sup> at highest flame temperature at the inlet of a direct fired fire tube. The most satisfactory design of firetube heating elements employs a zone by zone calculation based on thermal efficiency desired and limiting the maximum tube wall temperature as required by the solution to prevent thermal degradation. The average heat flux, Q/A, is a result of these calculations.
7. Reclaimers are not used in DEA systems.
8. Reboiler temperatures are dependent on solution conc. flare/vent line back pressure and/or residual CO<sub>2</sub> content required. It is good practice to operate the reboiler at as low a temperature as possible.
9. Canadian and Foreign Patented DEA Process.
10. B.L. Crynes and R.N. Maddox, Oil Gas J., p. 65-67, Dec. 15 (1969). The heats of reaction vary with acid gas loading and solution concentration.

## Chapter 7

10. J.I. Lee, F.D. Otto, and A.E. Mather, Can. GPA Research Seminar, Nov. 1972. The heats of reaction vary with acid gas loading and solution concentration.

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### Thermodynamics Table 7. RENon-NRTL, UNIQUAC, and WILson Parameter List

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To describe realistically the Gibbs energy, the ideal model is usually not sufficient and then there are many possibilities open for the choice of model. Some correlations that address liquid-phase non-idealities are RENon NRTL, UNIQUAC, and WILson. In the regular model a parameter for each pair of constituents of the phase is introduced. This "binary interaction" parameter (BIP) can also be given some physical significance by comparing with the difference in bond energies between like and unlike atoms. The parameter is multiplied with the fractions of the two constituents and thus the parameter gives no contribution when any of the fractions is zero. And when the components do not have interactions including like component interactions, the parameters are assumed to be ideal and a value of one is used.

At this time, DESIGN II does not store binary interaction parameters for any of the three correlations. However, they can be included to fine tune the model via [Inline Fortran: Activity Coefficient Equations Binary Interaction Parameter](#) or set of data [ChemTran: K-Value Options](#). If additional data is available ([ChemTran: Database Sources for VLE and LLE Data](#)), it is recommended to regress experimental VLE data via ChemTran ([ChemTran Correlating Mixture Data](#)).

In general, the model predictions and phase equilibrium tends to be very sensitive to the binary interaction parameters, so care should be taken to choose the best available literature equilibrium data that closely represent the process conditions. Details to set-up the DESIGN II simulation file to access the ChemTran generated data file can be found in [ChemTran File Access Commands](#).

#### NOTES:

RENon-NRTL, UNIQUAC, WILson are usually used for mixtures of organic chemicals (eg. alcohols, ketones, etc...). For further details visit [Thermodynamics Quick Guide](#).

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### Thermodynamics Table 8. GERG2008 Component Database List

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The following components are the ONLY ones supported for the simulation when the reference equation of state GERG2008 is used. Listed below are 21 real species grouped for use along with GERG2008. Note that only the three species noted below were added to the previous list of 18 components supported by earlier GERG2004 (as of Version 11.01). If other components NOT in this list are present then the program will emit a warning with "GERG2008".

DESIGN II ID#	NAME	FORMULA	
1	HYDROGEN	H2	
2	METHANE	CH4	
3	ETHANE	C2H6	
4	PROPANE	C3H8	
5	ISOBUTANE; 2-METHYLPROPANE	C4H10	
6	N-BUTANE	C4H10	
7	ISOPENTANE	C5H12	
8	N-PENTANE	C5H12	
10	N-HEXANE	C6H14	
11	N-HEPTANE	C7H16	
12	n-OCTANE	C8H18	
13	N-NONANE	C9H20	<b>Added in GERG2008</b>
14	N-DECANE	C10H22	<b>Added in GERG2008</b>
46	NITROGEN	N2	
47	OXYGEN	O2	
48	CARBON MONOXIDE	CO	
49	CARBON DIOXIDE	CO2	
50	HYDROGEN SULFIDE	H2S	<b>Added in GERG2008</b>
62	WATER	H2O	
1171	ARGON	AR	



1172

HELIUM

HE

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**Thermodynamics Table 9. REFPROP Component Database List**


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The following components are the ONLY ones supported for the simulation when REFPROP method is used. Listed below are 57 real species grouped for use with REFPROP. No other components from the main components list will be allowed for use with REFPROP.

DESIGN II ID#	NAME	FORMULA
1	HYDROGEN	H2
2	METHANE	CH4
3	ETHANE	C2H6
4	PROPANE	C3H8
5	ISOBUTANE; 2-METHYLPROPANE	C4H10
6	N-BUTANE	C4H10
7	ISOPENTANE	C5H12
8	N-PENTANE	C5H12
9	NEOPENTANE; 2,2-DIMETHYLPROPANE	C5H12
10	N-HEXANE	C6H14
11	N-HEPTANE	C7H16
12	N-OCTANE	C8H18
13	N-NONANE	C9H20
14	N-DECANE	C10H22
22	ETHYLENE	C2H4
23	PROPYLENE; PROPENE	C3H6
27	ISOBUTYLENE; 2-METHYLPROPENE	C4H8
38	CYCLOHEXANE	C6H12
40	BENZENE	C6H6
41	TOLUENE	C7H8
46	NITROGEN	N2
48	CARBON MONOXIDE	CO
49	CARBON DIOXIDE	CO2
50	HYDROGEN SULFIDE	H2S
51	SULFUR DIOXIDE	SO2
62	WATER	H2O
63	AMMONIA	NH3
1002	ACETONE	C3H6O
1012	ETHANOL	C2H6O
1021	METHANOL	CH4O
1043	DINITROGEN OXIDE	N2O
1052	R14	CF4
1053	RC318	C4F8
1055	R152A	C2H4F2
1056	R143A	C2H3F3

## Chapter 7

1060	FLUORINE	F2
1087	CARBONYL SULFIDE	COS
1099	R21	CHFCL2
1101	NITROGEN TRIFLUORIDE	NF3
1114	R23	CHF3
1122	R115	C2CLF5
1153	R11	CCL3F
1154	R22	CHCLF2
1155	R13	CCLF3
1156	CYCLOPROPANE; TRIMETHYLENE	C3H6
1159	ISOHEXANE; 2-METHYL PENTANE	C6H14
1171	ARGON	AR
1173	NEON	NE
1174	KRYPTON	KR
1176	R12	CCL2F2
1204	R134A	C2F4H2
1205	R123	C2CL2F3H
1224	R125	C2HF5
1241	R32	CH2F2
1242	R124	C2HCLF4
1243	R142B	C2H3CLF2
1273	R236EA	C3H2F6

### Thermodynamics: Unifac and LLE Unifac Specification Example

When VLE/LLE data is scarce or non-existent, the UNIFAC group contribution method can be used to estimate the non-ideal interactions between binary pairs of components. UNIFAC LLE group interactions are available for 32 different groups representing hydrocarbons, water, alcohols, organic acids, and other compounds. The correlation is considered accurate for temperatures between 30 and 125 C, and pressures between 1 and 3 atmospheres. For further details visit [Thermodynamics: K-Value Commands](#) and [Thermodynamics: Petro-Chemical and Chemical Process](#).

#### Using UNIFAC to Predict Both VLE and LLE

Since UNIFAC parameters are different for predicting VLE and LLE, the user must specify either UNIFACK or LL UNIFACK in the general section. If a flow sheet requires UNIFAC to estimate both VLE and LLE phase behavior, use either UNIFACK or LLUNIFACK as a general section command and specify the other using the KKEY = command in the unit operation where required. Both VLE and LLE parameter libraries may be specified in the general section. See the example input file below.

```
AB123.
* USE OF VLE AND LLE UNIFAC
  HEAt EXChanger 1 = E101, 1, -2
  TEMperature OUT = 100
  MULTiple PHase 2 = V101, 2, -3, -4, -5
C- Specify use of LLE UNIFAC parameters
  KKEY = LL UNIFACK
GENERAL SECTION
  COMponents = 62, 40, 41, 45
C- Specify use of VLE UNIFAC parameters
  UNIFACK
C- Load VLE and LLE UNIFAC parameters databanks
  VLE UNIFAC = 2
  LLE UNIFAC = 1
  FLOWrate 1 = 100, 100, 100, 100
  TP 1 = 70, 14.7
END
```

**NOTE:** For clarity, keywords are shown with their complete spellings using capitals and lowercase letters. Only those letters shown in CAPitals are actually required by DESIGN II. If complete keywords are used, they must be in all CAPITALS as DESIGN II is case sensitive and will not accept lowercase letters in input files.

## DESIGN II Modified Peng-Robinson Example Input

The following example shows how ChemTran is used to regress CO<sub>2</sub>-water VLE data to the modified Peng-Robinson method. A section of the associated DESIGN II file is shown.

```

AB123.
* CHEMTRAN input file to be used with DESIGN II input file.
C-           Water, CO2
COMPONENTS = 62, 49
C- Specify MODified PENG Robinson equation of state with MARGules mixing rule.
MODPENK (MARGULES)
C- Specify regression of Kappa parameters from library vapor pressure data KMODPEN (VAPOR) 62
KMODPEN (VAPOR) 49
C- Regress VLE data
P-X-Y (BAR,K) 49,62 = 383.15, 99.999,.0140,.9560,
                        199.997,.0210,.9580,
                        299.995,.0240,.9480,
                        399.994,.0260,.9320,
                        499.992,.0280,.9140,
                        599.991,.0300,.8930,
                        699.990,.0315,.8720,
                        799.988,.0330,.8540,
                        899.986,.0345,.8400,
                        1499.997,.0400,.8000,

P-X-Y (BAR,K) 49,62 = 423.15, 99.999,.0135,.8800,
                        199.997,.0215,.9100,
                        299.995,.0260,.9000,
                        399.994,.0290,.8820,
                        499.992,.0320,.8620,
                        599.991,.0345,.8400,
                        1499.997,.0480,.7520,

P-X-Y (BAR,K) 49,62 = 473.15, 99.999,.0130,.7150,
                        199.997,.0260,.8200,
                        299.995,.0340,.8250,
                        399.994,.0410,.8160,
                        499.992,.0470,.8000,
                        599.991,.0520,.7800,
                        999.985,.0630,.7200,

P-X-Y (BAR,K) 49,62 = 543.15, 599.991,.1060,.5460,
                        699.990,.1250,.5200,
                        799.988,.1450,.4960,
                        899.986,.1660,.4620,
                        1299.982,.2880,.2880

END

```

## Thermodynamics: References

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## Chapter 7

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# Chapter 8: Calculation Options

Several commands are available that you can use to ask for additional calculations which are performed independently of equipment calculations or to suppress certain calculations. These are listed as *Calculation Options in Flowsheet*. The calculation option commands are divided into four categories:

- execution control,
- stream (mixture) properties
- standard conditions, and
- LOST work.

## Calculation Options In Flowsheet

### Calculation Options: Execution Control

#### **CHEck INP**ut

This command is highly recommended for initial runs to avoid wasting time and money running a simulation with incorrect data. No equipment calculations are performed. The printout allows you to review input data and calculation order and also indicates any recycle streams (for which you should supply FLO and TP guesses).

#### **STOp =**

Enter the equipment number after which you wish calculations to stop. Results will be printed for all equipment modules and streams calculated up to that point. This command can be used to slowly work through a complicated flowsheet one step at a time. Also the STOP command can be used like the CHEck INP command. The STOP command would be particularly useful when equipment modules exist that could be calculated before the recycle is reached. By calculating these front-end equipment modules, information useful in guessing recycles might be obtained.

#### **MAT**erial **BAL**ance

Enter this command when you only want a material balance calculation performed. No heat balance calculation will be attempted.

The following equipment modules can be used with the following restrictions:

#### **COM**ponent **SPL**itter

RECOvery TOP in mass or molar units, no TEMperature commands, no HKE or KKE.

#### **CON**Troller

No ENThalpy, VAPor FRAction, or TEMperature OUT.

#### **DIV**ider

FLOw RATE specified in mass or molar units, no HKE or KKE commands.

#### **MIX**er

No HKE or KKE commands.

#### **STR**eam manipulator

No SCF/MOL, HKE or KKE commands, no HEAt VALue calculation,

**NOTE:** None of the following modules are allowed in the flowsheet when using MATerial BALance:

<b>REF</b> ine	<b>DIS</b> tillation
<b>FLA</b> sh	<b>VAL</b> ve with phase separation

All flows will be reported as liquid.

### Calculation Options: Stream (Mixture) Properties

#### **LAT**ent **HEA**t of **VAP**orization

Calculates the latent heat of vaporization of a mixture with one or more species in a multi-phase stream.

#### **CAL**culate **BUB**ble point = s1, s2, s3, or ALL

Calculates the bubble point temperature for the specified stream(s).

#### **CAL**culate **DEW** point = s1, s2, s3, or ALL

Calculates the dew point temperature for the specified stream(s).

#### **CAL**culate **VAP**or **PRE**ssure = s1, s2, s3, or ALL

Calculates the vapor pressure for the specified stream(s).

#### **CAL**culate **WAT**er dew point = s1, s2, s3, or ALL

Calculates the water dew point temperature for the specified stream(s). The method for determining water dew point will be consistent with the thermodynamic commands specified in the GENeral section. This feature may only be used when water is declared immiscible. (IMM = 62).

#### **CAL**culate phase **MAP** curve = s1, s2, s3, or ALL

Calculates the phase map curves with bubble, dew and critical points for the specified stream(s). No immiscible water allowed.

## Chapter 8

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### **CAL**culate phase **ENV**elope curve = s1, s2, s3, or ALL

Calculates the phase envelope curves bubble, dew and critical points for the specified stream(s). Immiscible water is allowed.

### **CAL**culate **PVH PRE**ssure (P units) j = P1, P2,...P100

Calculates the pressure versus enthalpy curves for pressures (P1,...) up to 100 data points, where "j" is the stream number or the word ALL.

### **CAL**culate **PVH TEM**perature (T units) j = T1, T2,...T10

Calculates the pressure versus enthalpy curves for isotherm temperatures (T1,...) up to 10 data points, where "j" is the stream number or the word ALL.

#### **NOTES:**

1. If the P-H diagram is generated then a phase envelope diagram will be automatically generated first.
2. If the user does not put in pressures then the pressures will be automatically generated starting at 14.7 psia, 50 psia, 100 psia, 150 psia and up to 120% of the top pressure for the bubble point or dew point.
3. If the user does not put in isotherm temperatures then seven isotherm temperatures will be generated from the lowest bubble point temperature to 120% of the highest dew point temperature.

### **CAL**culate **PVS PRE**ssure (P units) j = P1, P2,...P100

Calculates the pressure versus entropy curves for pressures (P1,...) up to 100 data points, where "j" is the stream number or the word ALL.

### **CAL**culate **PVS TEM**perature (T units) j = T1, T2,...T10

Calculates the pressure versus entropy curves for isotherm temperatures (T1,...) up to 10 data points, where "j" is the stream number or the word ALL.

### **CAL**culate **PVD PRE**ssure (P units) j = P1, P2,...P100

Calculates the pressure versus density curves for pressures (P1,...) up to 100 data points, where "j" is the stream number or the word ALL.

### **CAL**culate **PVD TEM**perature (T units) j = T1, T2,...T10

Calculates the pressure versus density curves for isotherm temperatures (T1,...) up to 10 data points, where "j" is the stream number or the word ALL.

#### **AIR FIX OFF**

Replacing AIR (ID#99) with 79 mol% Nitrogen (ID#46) and 21 mol% Oxygen (ID#47) will not be done (found in **Specify...Preferences** dialog).

### **CAL**culate **MEN** methane number = s1, s2, s3, or ALL

Calculates the methane number for the specified stream(s). This feature is automatically turned on for all streams and the results can be found in the detailed stream print. The method for determining the same is provided in this link <http://www.arb.ca.gov/regact/cng-lpg/appd.PDF>.

### **CAL**culate **WOB**be index = s1, s2, s3, or ALL

Calculates the wobbe index or number for the specified stream(s). It is the gross heating value of a gas divided by the square root of its gravity. The gas gravity is the relative gas density (to air) at 0 degrees C and 1 atm.

### **CAL**culate gross **HEA**ting value = s1, s2, s3, or ALL

Enter this command to get the gross heating value calculated for specified hydrocarbon stream(s). Gross heating value assumes all water is fully condensed.

### **CAL**culate **NET HEA**ting value = s1, s2, s3, or ALL

Enter this command to get the net heating value calculated for a specified hydrocarbon stream(s). Net heating value assumes water leaves in the stream without being condensed.

#### **NOTES:**

1. The difference between NET and GROSS heating value is the latent heat of condensation of the water vapor present in the hydrocarbon stream.
2. DESIGN II has gross heating values for most components and net heating value for 65 components (Fig. 23-2 of page 23-4 in GPSA manual). Net heating values for components not covered by data are estimated from gross heating values by subtracting water latent heats for estimated amount of water produced. DESIGN II also estimates heating values for petroleum fractions/cuts. You may enter HIGH and LOW HEATING values for petroleum fractions, or an estimate for CARBON to HYDROGEN weight ratio for calculating the gross heating value.

### **SAT**urate **FEE**ds **WAT**er = n1,n2,n3, or ALL

n1,n2,n3, etc. are feed stream numbers. DESIGN II will automatically saturate the specified or ALL feed streams with water. The method for determining water saturation will be consistent with the thermodynamic commands specified in the GENERAL section. This feature may only be used when water is declared immiscible. (IMM = 62 or appropriate density value option)

### **SON**ic velocity of **STR**eams = s1, s2, s3, or ALL

Calculates the sonic velocity for the specified vapor stream(s).

### **CO2 FRE**eze =

Enter the stream number(s) for which you want DESIGN II to check for formation of solid CO<sub>2</sub>. Enter stream numbers in ascending order. For CO<sub>2</sub> FREeze calculation for all streams, specify ALL after the equals sign. Add a CO<sub>2</sub> FREeze command to the DIStillation column calculation to check for CO<sub>2</sub> freezing on trays. See Distillation: Calculation Options for additional information about this command.

DESIGN II will predict the conditions at which hydrate formation will occur for any stream in the process simulation. Locate these commands in the GENeral section of the input file.

### TEMperature of HYDrate formation =

Enter the stream numbers, in any order, to be checked for hydrate formation or ALL to check all streams. DESIGN II will predict the temperature at which hydrates will form at the stream pressure.

### PREssure of HYDrate formation =

Enter the stream numbers, in any order, to be checked for hydrate formation or ALL to check all streams. DESIGN II will predict the pressure at which hydrates will form at the stream temperature.

DESIGN II will predict critical temperature and pressures for natural gas streams with the following command.

### CALculate HYDrate curve = s1, s2, s3, or ALL

Calculates the hydrate curves for the specified stream(s).

### CRITical PROperties =

Enter the stream number(s) of natural gas mixtures for which you want critical temperature and pressure calculated. **Enter stream numbers in ascending order.** ALL after the equals sign will have T<sub>c</sub> and P<sub>c</sub> calculated for every stream in your simulation. The results are printed in the detailed stream summaries for the specified streams.

**NOTE:** This calculation is valid only for light natural gas streams- methane, ethane, propane, etc., plus a reasonable amount of nitrogen, carbon dioxide and hydrogen sulfide. The specified streams should contain no water.

### Reid Vapor Pressure

Four different options are available for Reid Vapor Pressures calculations for mixtures: ASTM D323-94 is employed for REID and REI AST commands. REI CRU command uses API Technical Data Book procedure 5B1.2 (crude feeds-ASTM D323-79), and REI PRO command uses procedure 5B1.1 (finished products-ASTM D323-79). You may choose one method per stream. REID and REI AST methods will be performed ONLY if Nitrogen (component id number 46) is present in the component list of the GENeral section. Other methods (REI CRUde, REI PROducts) are NOT required to have Nitrogen in the component list. The API 5B1.1 REI PROducts method, requires a crude feed description or section. The thermodynamic option KVAL is not permitted when calculating Reid Vapor Pressure. If KVAL is chosen, the Reid Vapor Pressure calculation is bypassed.

### REID vapor pressure =

Enter the individual or ALL stream number(s) of hydrocarbon streams (natural gas and crude oils) for which you want the Reid vapor pressure (RVP) calculated. DESIGN II will calculate the Reid vapor pressure(s) in accordance with ASTM D323-94\*. The results will be printed in the detailed stream summaries for the specified streams. A calculation method label will be included in the report.

### REI AST =

Enter, **in ascending order**, the number(s) of hydrocarbon streams (natural gas and crude oils) for which you want the Reid vapor pressure (RVP) calculated. DESIGN II will calculate the Reid vapor pressure(s) in accordance with ASTM D323-94\*. The results will be printed in the detailed stream summaries for the specified streams. A calculation method label will be included in the report. This is also the default method for the **REID** vapor pressure command.

\* Requires Nitrogen (component id number 46) to be present in the component list

### REI CRUde =

Enter, in ascending order, the numbers of the hydrocarbon streams (crude feeds) for which you want the Reid vapor pressure calculated. DESIGN II will calculate the Reid vapor pressure in accordance with API Technical Data Book procedure 5B1.2. The results will be printed in the detailed stream summaries for the specified streams. A calculation method label will be included in the report.

### REI PROducts =

Enter, in ascending order, the numbers of the hydrocarbon streams (finished products for which you want the Reid vapor pressure calculated. DESIGN II will calculate the Reid vapor pressure in accordance with API Technical Data Book procedure 5B1.1. The results will be printed and labeled with the calculation method in the detailed stream summaries for the specified streams.

### REI ASTMA =

Enter, in ascending order, the numbers of the hydrocarbon streams (gasoline and other petroleum products with a vapor pressure of less than 26 psi or 180 KPA). DESIGN II will calculate the Reid vapor pressure in accordance with Procedure A of ASTM D323. The results will be printed and labeled with the calculation method in the detailed stream summaries for the specified streams.

### REI ASTMC =

Enter, in ascending order, the numbers of the hydrocarbon streams (gasoline and other petroleum products with a vapor pressure greater than 26 psi or 180 KPA). DESIGN II will calculate the Reid vapor pressure in accordance with Procedure

## Chapter 8

---

C of ASTM D323. The results will be printed and labeled with the calculation method in the detailed stream summaries for the specified streams.

### Example

**COM** = 62, 46, 2, 3, 49, 50, 4, 5, 6, 7, 8  
**REI AST** = 1  
**REI CRU** = 2, **REI PRO** = 3, 4, 5, 6

### COOLing CURve j

Enter this command to get a cooling curve from the stream temperature to the bubble point, where "j" is the stream number.

### COOLing CURve (T units,P units) j =

Enter the temperature change, pressure change, and number of increments for stream number "j" cooling curve calculation. Starting temperature and pressure are stream conditions.

### HEAting CURve j

Enter this command to get a heating curve for stream "j" from the stream temperature to the dewpoint, where "j" is the stream number.

### HEAting CURve (T units, P units) j =

Enter the temperature change, pressure change, and number of equal temperature increments you want calculated for the heating curve for stream "j", where "j" is the stream number.

**NOTE:** For COOLing CURve calculations, if the stream temperature is below the bubble point, DESIGN II will calculate a heating curve instead. Conversely, if the stream temperature is above the dewpoint for a HEAting CURve, a cooling curve will be calculated.

### CONdensate RECover =

Enter the feed stream number(s) and liquid product stream number(s) for which the calculation is to be performed. Product stream numbers should be entered as negative values. DESIGN II will calculate the gallons of liquid condensate per 1000 standard cubic feet (MSCF) of total feed for each liquid product stream specified. The liquid for each component will be reported as gallons per 1000 standard cubic feet (MSCF) of feed. The total value reported will be the total gallons of condensate per total MSCF of feed. The feed streams will be combined for the calculation if more than one feed stream is specified.

### BULK = s1, s2, s3, or ALL

Enter the stream numbers feeding to Heat Exchangers (shell & tube, air-cooler, plate-fin), LNG Exchangers, and for Distillation Column internal heat exchangers for which cooling/heating curves be printed out in the detailed stream summary section. DESIGN II will also report additional parameters such as phase limit temperatures, physical and thermodynamic properties for each of the phases occurring.

---

## Calculation Options: Standard Conditions

---

### AMBient PREssure =

Enter the ambient pressure. Units are PSIA. DESIGN II allows direct entry of pressure specifications in gauge units. If the ambient pressure is not 14.696 PSIA (sea level), use this command in the GENeral section. Any pressure entered as PSIG is converted to PSIA in DESIGN II by adding the ambient pressure as follows: **PSIG + ambient pressure = PSIA**

### Example

**PREssure OUT** (PSIG) = 100  
**GENeral**  
**AMBient PRE**= 14.5  
**TP** (PSIG) 1 = 100,1250

### API ENTHALPY

Prints stream enthalpy / entropy using -200 F saturated liquid base per API.

### ASME ENTHALPY

Prints stream enthalpy / entropy using 32 F saturated liquid base per ASME.

Note : If both API and ASME enthalpy base options are selected then all components except water will be printed using a -200 F saturated liquid base. Water will be printed at 32 F saturated liquid base.

### GERG ENTHALPY

Prints stream enthalpy / entropy using 77 F (298.15 K or 25 C) ideal gas base per GERG.

DESIGN II allows definition of the standard conditions for reporting product volumetric flows (MMSCF and GPM). Specify the STAndard PREssure and STAndard TEMperature with the following commands in the GENeral section. This option is available only when the default output pressure and temperature units are used. Default standard conditions are 60 F and 14.696 PSIA.

### STAndard PREssure (P units) =

Enter the pressure for volume calculations at standard conditions with default output units. The default is 14.696 PSIA.

### STAndard TEMperature (T units) =

Enter the temperature for volume calculations at standard conditions with default units. The default is 60 F.

For metric and SI units use **NORmal PREssure** and **NORmal TEMperature** commands in the **GENeral** section to adjust conditions for standard volume calculations. NTP conditions are 0 C and 1 Atmosphere.

**NORmal PREssure (P units) =**

Enter the pressure for volume calculations at standard conditions with metric and SI units. The default is 1 atm.

**NORmal TEMperature (T units) =**

Enter the temperature for volume calculations at standard conditions with metric and SI units. The default is 0 C.

---

### Calculation Options: Heat Exchanger Temperature Crossover

---

If a temperature crossover is identified by the program in a heat exchanger, the program will now recalculate the heat exchanger with a default temperature approach specification of 5 F. Warning messages will be printed for the users information. The command to allow temperature crossovers that bypasses this recalculation should be placed in the **GENeral** section (Specify...Preferences for dialog activation) and it is as follows:

**HXCROSS ALLOWED**

Enter this command to allow temperature crossovers in all heat exchanger(s) on the flowsheet.

---

### Calculation Options: Lost Work

---

**LOSt work**

Enter this command in the **GENeral** section. The **LOSt work** analysis combines the First and Second Laws of Thermodynamics to measure the thermodynamic efficiency of a process. Using the availability function and the heat and work exchanged, the program can calculate the lost work of equipment at specified conditions.

$$\text{Lost Work} = \text{Bin} - \text{Bout} + (1 - \text{Tamb}/\text{Texchange}) * \text{Q} - \text{W}$$

where

Bin and Bout are the availability functions of streams. (availability function = Enthalpy - (Tamb\*Entropy)

Tamb is the ambient temperature in absolute units

Texchange is the exchange temperature in absolute units

Q is heat transferred into or from the equipment

W is external work

Lost work analysis will not be performed for **CONTRoller**, **DIVider**, **isothermal FLAsh**, **MULTiple FLAsh**, **MULTiple PHAse flash**, **PHAse envelope**, **PHAse MAP**, **STReam manipulator**, **HYdroTREater** or **REFIne** modules.

**NOTE:** Lost work analysis for **REActor** modules requires **HEAt of FORmation** and **ENTropy of FORmation** for all components with ID numbers greater than 99. See **THERMODYNAMICS** Section for details.

Several optional commands exist that override the default exchange temperatures or ambient temperature. These commands are primarily used for heat exchange calculations where only the process side has been defined (e.g. single stream **HEAt EXChanger**). These commands must be placed in the **GENeral** section.

**TEMperature of AMBient (T units) =**

Enter ambient temperature. Default is 77F.

**TEMperature of HEAting fluid (T units) =**

Enter heating medium temperature. Default is 250F.

**TEMperature of COOLing fluid (T units) =**

Enter cooling fluid temperature. Default is 70.3 F.

**TEMperature of REFrigerant (T units) =**

Enter refrigerant temperature. Default is -100 F.

The equipment modules which have commands for changing exchange temperatures are **COMPRe** (with multiple **STAGes**), **DIStillation**, **FIRed heater**, **FLAsh** (with **HEA =**), **HEAt EXChanger**, **REActor** and **SHORtcut fractionator**. See the corresponding **Equipment Modules** for details.

---

### Calculation Options: Dynamic Simulation

---

**TIMe STEp (t units)**

Enter the time step for the dynamic simulation. Default is 5 minutes.

**TIMe DURation (t units)**

Enter the time duration for the dynamic simulation. Default is 60 minutes.

If these two commands are present, then **DESIGN II** for Windows will automatically shift itself into dynamic mode from steady state mode.

## Calculation Options Command Summary

**Dynamic Simulation**

**Standard Conditions**

## Chapter 8

**TIME STEP**

**TIME DURATION**

### Execution Control

**CHECK INPUT**

**STOP =**

**MATERIAL BALANCE** (Note: No Heat Balance calculation will be attempted)

### Heat Exchanger Temperature Crossover

**HXCROSS ALLOWED**

### Stream (Mixture) Properties

**LATENT HEAT VAPORIZATION**

**CALCULATE BUBBLE POINT =**

**CALCULATE DEW POINT =**

**CALCULATE VAPOR PRESSURE =**

**CALCULATE WATER DEW POINT =**

**CALCULATE PHASE MAP CURVE =**

**CALCULATE PHASE ENVELOPE CURVE =**

**CALCULATE PVH PRESSURE =**

**CALCULATE PVH TEMPERATURE =**

**CALCULATE PVS PRESSURE =**

**CALCULATE PVS TEMPERATURE =**

**CALCULATE PVD PRESSURE =**

**CALCULATE PVD TEMPERATURE =**

**AIR FIX OFF**

**CALCULATE MEN METHANE NUMBER =**

**CALCULATE WOBBE INDEX =**

**CALCULATE GROSS HEATING VALUE =**

**CALCULATE NET HEATING VALUE =**

**SATURATE FEEDS WATER =**

**SONIC VELOCITY OF STREAM =**

**CO2 FREEZE =**

**AMBIENT PRESSURE =**

**STANDARD PRESSURE (P UNITS) =**

**STANDARD TEMPERATURE (T UNITS) =**

**NORMAL PRESSURE (P UNITS) =**

**NORMAL TEMPERATURE (T UNITS) =**

### Stream (Mixture) Properties

**TEMPERATURE OF HYDRATE FORMATION =**

**PRESSURE OF HYDRATE FORMATION =**

**CALCULATE HYDRATE CURVE =**

**CRITICAL PROPERTIES =**

**REID VAPOR PRESSURE =**

**REID AST =**

**REID CRUDE =**

**REID PRO =**

**STEAM TABLES**

**COOLING CURVE X**

**COOLING CURVE (T UNITS, P UNITS) X =**

**HEATING CURVE X**

**HEATING CURVE (T UNITS, P UNITS) X =**

**CONDENSATE RECOVERY =**

**BULK =**

### Lost Work

**LOST WORK**

**TEMPERATURE OF AMBIENT (T UNITS) =**

**TEMPERATURE OF HEATING FLUID (T UNITS) =**

**TEMPERATURE OF COOLING FLUID (T UNITS) =**

**TEMPERATURE OF REFRIGERANT (T UNITS) =**

## Calculation Options Step by Step

### Calculation Options Step 1

**Execution control commands. Select any of the GENERAL section calculation option commands listed below:**

Check input for coding errors (no program execution)

Stop after specified equipment number

Perform material balance calculation only (no heat balance calculation will be attempted)

**CHE INP**

**STO =**

**MAT BAL**

### Calculation Options STEP 2

**Stream (Mixture) property commands. Select any of the GENERAL section stream mixture properties listed below:**

Stream number(s), in ascending order to calculate the bubble point of streams or **ALL** after the equals sign to check all streams

**CAL BUB =**

Stream number(s), in ascending order to calculate the dew point of streams or **ALL** after the equals sign to check all streams

**CAL DEW =**

Stream number(s), in ascending order to calculate the vapor pressure of streams or **ALL** after the equals sign to check all streams

**CAL VAP PRE=**

Stream number(s), in ascending order to calculate the water dew point of streams with water or **ALL** after the equals sign to check all streams

**CAL WAT =**

Stream number(s), in ascending order to calculate the wobbe index or number for the streams or **ALL** after the equals sign to check all streams

**CAL WOB =**

Stream number(s), in ascending order to calculate the GROSS heating value for the streams or **ALL** after the equals sign to check all streams

**CAL HEA =**

Stream number(s), in ascending order to calculate the NET heating value for the streams or **ALL** after the equals sign to check all streams

**CAL NET HEA =**

Stream number(s), in ascending order to check for saturating feed streams with water or **ALL** after the equals sign to check all streams

**SAT FEE WAT =**

Stream number(s), in ascending order to calculate the sonic velocity of vapor streams or **ALL** after the equals sign to check all streams

**SON STR =**

Stream number(s), in ascending order to check for formation of solid CO2 or **ALL** after the equals sign to check all streams

**CO2 FRE =**

Stream number(s), in any order, to predict hydrate formation temperature or <b>ALL</b> after the equals sign to check all streams	<b>TEM HYD =</b>
Stream number(s), in any order, to predict hydrate formation pressure or <b>ALL</b> after the equals sign to check all streams	<b>PRE HYD =</b>
Stream number(s), in ascending order, of natural gas mixtures for critical temperature and pressure calculation or <b>ALL</b> after the equals sign to check all streams (valid only for light natural gas streams)	<b>CRI PRO =</b>
Stream number(s), in ascending order, of hydrocarbon streams (natural gas and crude oils) for Reid vapor pressure (RVP) calculation (Nitrogen, ID number 46, must be present in the component list in the <b>GENeral</b> section)	<b>REID =</b>
Use the NBS/NRC steam tables in process simulation for any pure water stream	<b>STE TAB</b>
Cooling curve from the stream temperature to the bubble point where "j" is the stream number; 10 equal temperature increments with no pressure change	<b>COO CUR j</b>
Temperature change, pressure change and number of increments entered after equals sign and separated by commas for stream number "j" cooling curve	<b>COO CUR (T units, P units)</b>
Heating curve for stream "j" from the stream temperature to the dewpoint, where "j" is the stream number	<b>j =</b> <b>HEA CUR j</b>
Temperature change, pressure change, and number of increments entered after equals sign and separated by commas for stream number "j" heating curve	<b>HEA CUR (T units, P units) j</b>
Feed stream number(s) and liquid product stream number(s) for calculation of gallons of liquid condensate per 1000 standard cubic feet (MSCF) (product stream numbers should be entered as negative values)	<b>=</b> <b>CON REC =</b>
Enter the stream numbers feeding to Heat Exchangers, LNG Exchangers, and for Distillation Column internal heat exchangers for which cooling/heating curves be printed out in the detailed stream summary section. <b>DESIGN II</b> will also report additional parameters such as phase limit temperatures, physical and thermodynamic properties for each of the phases occurring.	<b>BULK =</b>

### English units standard conditions commands

Ambient pressure (units are PSIA)	<b>AMB PRE =</b>
Standard pressure for volume calculations with default output units; default is 14.696 PSIA	<b>STA PRE (P units) =</b>
Standard temperature for volume calculations with default units; default is 60 F	<b>STA TEM (T units) =</b>

### Metric and SI units standard conditions commands

Normal pressure for volume calculations with metric and SI units (default is 1 atm)	<b>NOR PRE (P units) =</b>
Normal temperature for volume calculations with metric and SI units (default is 0 C)	<b>NOR TEM (T units) =</b>

---

## Calculation Options STEP 3

---

### Lost work commands. Select any of the LOST work options listed below:

Calculate the lost work of equipment and streams at specified conditions	<b>LOS</b>
Ambient temperature (default is 77 F)	<b>TEM AMB (T units) =</b>
Heating medium temperature (default is 250 F)	<b>TEM HEA (T units) =</b>
Cooling fluid temperature (default is 70.3 F)	<b>TEM COO (T units) =</b>
Refrigerant temperature (default is -100 F)	<b>TEM REF (T units) =</b>

## Calculation Options Examples

---

### Calculation Options: Calculate Dew/Bubble Points, Heating Values & Wobbe Index

---

A sample input file and the output from a detailed stream summary are shown below. The dew point temperature, bubble point temperature, water dew point temperature, heating (gross and net) values and Wobbe index are calculated for the specified streams in the input section (stream dialog...calculation options).

#### Coding

```

AB123.
*Calculate Dew/Bubble Points, Heating Values & Wobbe Index

C- EQUIPMENT MODULES

HEA EXC 1 = E-400-1, 1,-2,
U (BTU/HR/FT2/F) = 50.
TEM OUT(F) = 104.
SHE PAS = 1
TUB PAS = 1
SHE = 1
TUB FEE = 1
INL = OPP
HOR
    
```

# Chapter 8

```

DEL(P5I) = 0.

FLA 2 = V-160, 2,-3,-4,

C- GENERAL SECTION
GENERAL
COMPONENTS = 62,50,46,49,2,3,4,5,6,7,8,10,
APISOAVEK
APISOAVEH
STDD
VIS VAP = MODAPI
VIS LIQ = MODAPI
THE CON LIQ = TEMA
SUR TEN = STD
PRE UNI OUT = PSIG
MAX = 1
CON TOL = 1.E-003
FLO(LBMOL/HR)1 = 22.35,0.29,0.11,55.62,113.53,118.2,285.84,110.687,146.724,
55.5284,50.8802,24.971,
TP (F,PSIG) 1 = 60.,80.
NAM STR 1 = Strm 1
NAM STR 2 = Strm 2
NAM STR 3 = Strm 3
NAM STR 4 = Strm 4
CALCulate gross HEATING value = 1, 3, 4
CALCulate NET HEATING value = 1, 3, 4
CALCulate WOBbe index = 1, 3, 4
CALCulate WATER dew point = ALL
CALCulate DEW point = ALL
CALCulate BUBble point = ALL
END

```

A portion of the output generated by the above input file follows.

STREAM NUMBER	1	CONNECTING	( 0)	FEED			
NAME:	Strm 1	TO	( 1)	E-400-1			
ASOA K-VALUES	ASOA ENTHALPY	STD	DENSITY	FLOW RATES /HR			
COMPONENT NAME	TOTAL LBMOL	LIQUID LBMOL	VAPOR LBMOL	TOTAL LB	TOTAL MOL PCT	KVALUE	
WATER	22.3500	0.222036	1.54003	402.643	2.2697	6.5434	
H2S	0.290000	0.061795	0.228205	9.88320	0.029450	3.4839	
NITROGEN	0.110000	0.001282	0.108718	3.08147	0.011171	79.999	
CO2	55.6200	4.97030	50.6497	2447.83	5.6482	9.6138	
METHANE	113.530	4.49964	109.030	1821.36	11.529	22.860	
ETHANE	118.200	22.4087	95.7913	3554.04	12.003	4.0328	
PROPANE	285.840	130.636	155.204	12603.8	29.027	1.1208	
I-BUTANE	110.687	75.1897	35.4973	6433.13	11.240	0.44539	
N-BUTANE	146.724	110.155	36.5692	8527.60	14.900	0.31319	
I-PENTANE	55.5284	49.2141	6.31428	4006.15	5.6389	0.12104	
N-PENTANE	50.8802	46.4087	4.47149	3670.80	5.1669	0.090897	
N-HEXANE	24.9710	24.2663	0.704673	2151.80	2.5358	0.027396	
TOTAL	984.731	468.033	496.109	45632.1	100.000		
TOTAL LB	45632.1	26493.2	18768.0				

```

STREAM NUMBER 1
TEMPERATURE DEG F 60.000
PRESSURE PSIG 80.000
ENTHALPY BTU/HR -4.27107E+06
VAPOR FRACTION 0.50380

```

PROPERTIES	TOTAL	VAPOR	LIQUID *	WATER
FLOWRATE LBMOL/HR	984.7305	496.1094	468.0333	20.588
MOLECULAR WT.	46.3397	37.8304	56.6054	18.015
ENTHALPY BTU/LBMOLE	-4337.2979	172.5516	-8479.0234	-18856.063
ENTROPY BTU/LBMO/R	-7.1981	0.289439	-14.2139	-28.133
CP BTU/LBMO/R		15.3123	32.8752	17.348
CV BTU/LBMO/R		12.7062	25.8549	
CP/CV		1.2051	1.2715	
DENSITY LB/FT3		0.692688	35.1346	62.383
Z-FACTOR		0.927487	0.027361	0.4904E-02
FLOWRATE FT3/SEC T-P		7.5262		
GAL/MIN T-P			94.0174	0.741
MMSCFD STP		4.5177		
S.G. (TS/60) GPA STP			0.568485	1.000



```

VISCOSITY CP 0.9326E-02 0.171902 1.122
TH.COND BTU/FT/HR/F 0.012087 0.087670 0.341
SURFACE TENSION DYNE/CM 11.2409 73.285
HEATING VALUE (GROSS) BTU/SCF 2465.7
HEATING VALUE (NET) BTU/SCF 2269.1
WOBBE NUMBER BTU/SCF 1930.5
WATER DEW POINT F 125.34
DEW POINT TEMPERATURE F 124.26
BUBBLE POINT TEMPERATURE F -109.30
    
```

```

* LIQUID PROPERTIES CALCULATION EXCLUDING FREE WATER
  TS IS STANDARD TEMPERATURE AT 60.00 DEG F
    
```

## Calculation Options: Checking For CO2 Freeze-Up

Solid CO<sub>2</sub> formation is an important problem in cryogenic processing as precipitation of solid CO<sub>2</sub> may reduce process efficiency and, in many cases, foul process equipment. DESIGN II has a reliable prediction technique for formation of CO<sub>2</sub> solids in light hydrocarbon mixtures. One of the following messages will print in the detailed stream summaries when you specify this option:

A check for CO<sub>2</sub> freezing for streams 2, 5, and 10 of a simulation is performed if the following command is entered in the GENERAL section:

```
CO2 FREEZE = 2,5,10
```

A portion of the output file is shown below:

```

** TEST CO2 FREEZE-UP FOR STREAM 2
*****
***NO CO2 FREEZE-UP IS INDICATED ***
*****
** TEST CO2 FREEZE-UP FOR STREAM 5
*****
*** WARNING: CO2 FREEZE-UP IS PREDICTED ***
*****
** TEST CO2 FREEZE-UP FOR STREAM 10
*****
*** WARNING: CO2 FREEZE-UP REGION IS APPROACHED ***
*****
    
```

## Calculation Options: Hydrate Formation Prediction

A sample input and the output from a detailed stream summary are shown below. The temperature of hydrate formation at stream pressure and the pressure of hydrate formation at stream temperature were requested in the input section.

```

*HYDRATE FORMATION
FLASH 1 = DUM, 1,-2, -3
GENERAL
  COMPONENTS = 2,3,4,5,6,11,46,62
  TEMPERATURE OF HYDRATE FORMATION = 2,3,
  PRESSURE OF HYDRATE FORMATION = ALL
  FLOW 1 = 8641,647,357,99,114,78,64,400
  TP 1 = 71.5, 1779
  SOAVEK, SOAVEH, STDD
    
```

END

A portion of the output generated by the above input file follows.

```

HYDRATE FORMATION PAGE 11
          SOLUTION REACHED
STREAM NUMBER 2 CONNECTING ( 1) DUM
NAME:          TO ( 0) PRODUCT
SOAV K-VALUES  SOAV ENTHALPY  STD DENSITY  FLOW RATES /HR

COMPONENT NAME  TOTAL LIQUID VAPOR TOTAL TOTAL
                LBMOL LBMOL LBMOL LB MOL PCT KVALUE
-----
METHANE         8641.00  0.  8641.00  138627.  86.304
ETHANE          647.000  0.  647.000  19454.0  6.4620
PROPANE         357.000  0.  357.000  15741.6  3.5656
I-BUTANE        99.0000  0.  99.0000  5753.88  0.98878
N-BUTANE        114.000  0.  114.000  6625.68  1.1386
N-HEPTANE       78.0000  0.  78.0000  7815.44  0.77904
NITROGEN        64.0000  0.  64.0000  1792.86  0.63921
WATER           12.3089  0.  12.3089  221.749  0.12294
-----
TOTAL           10012.3  0.  10012.3  196033.  100.000
TOTAL LB       196033.  0.  196033.
    
```

# Chapter 8

```

STREAM NUMBER      2
TEMPERATURE DEG F      71.500
PRESSURE PSIA      1779.0
ENTHALPY BTU/HR      -1.01493E+07
VAPOR FRACTION      1.0000
    
```

```

PROPERTIES          TOTAL          VAPOR
-----
FLOWRATE LBMOL/HR  10012.3086  10012.3086
MOLECULAR WT.      19.5792    19.5792
ENTHALPY BTU/LBMOLE -1013.6838 -1013.6838
ENTROPY BTU/LBMO/R  -9.5738    -9.5738
CP BTU/LBMO/R      16.8888
CV BTU/LBMO/R      9.0747
DENSITY LB/FT3     8.4596
Z-FACTOR           0.722412
FLOWRATE FT3/SEC T-P 6.4369
                   MMSCFD STP  91.1747
VISCOSITY CP       0.017731
TH.COND BTU/FT/HR/F 0.029385
HYDRATE FORMATION PREDICTED AT STREAM TEMP. AND PRES. ABOVE 1752.1 PSIA
HYDRATE FORMATION PREDICTED AT STREAM PRES. AND TEMP. BELOW 71.615 DEG F

VISCOSITY CALCULATED BY METHOD OF ELY AND HANLEY (NBS81)
TS IS STANDARD TEMPERATURE AT 60.00 DEG F
    
```

## Calculation Options: Heating Curve

### General,

```

HEATING CURVE 7 = 100, 10, 15
COOLING CURVE 8
COOLING CURVE (C, BAR) 10 = 25, 1, 10
    
```

Output is shown on following pages.

```

STREAM NUMBER      7
    
```

```

+++ HEATING CURVE +++
TOTAL FLOW RATE = 968.29 LBMOL/HR
ENTERING ENTHALPY: 1.89474E+06 BTU/HR
    
```

	TEMPERATURE	PRESSURE	L/F	ENTHALPY		BTU/HR	HEATING DUTY
	F	PSIG		VAPOR	LIQUID		
1	136.48	4.4012	0.0000	1.8947E+06	0.0000E+00	0.0000E+00	0.0000E+00
2	143.14	3.7345	0.0000	2.0316E+06	0.0000E+00	0.0000E+00	1.3683E+05
3	149.81	3.0679	0.0000	2.1694E+06	0.0000E+00	0.0000E+00	2.7467E+05
4	156.48	2.4012	0.0000	2.3083E+06	0.0000E+00	0.0000E+00	4.1353E+05
5	163.14	1.7345	0.0000	2.4482E+06	0.0000E+00	0.0000E+00	5.5342E+05
6	169.81	1.0679	0.0000	2.5891E+06	0.0000E+00	0.0000E+00	6.9433E+05
7	176.48	0.40119	0.0000	2.7310E+06	0.0000E+00	0.0000E+00	8.3628E+05
8	183.14	-0.26548	0.0000	2.8740E+06	0.0000E+00	0.0000E+00	9.7926E+05
9	189.81	-0.93215	0.0000	3.0180E+06	0.0000E+00	0.0000E+00	1.1233E+06
10	196.48	-1.5988	0.0000	3.1631E+06	0.0000E+00	0.0000E+00	1.2684E+06
11	203.14	-2.2655	0.0000	3.3092E+06	0.0000E+00	0.0000E+00	1.4145E+06
12	209.81	-2.9321	0.0000	3.4564E+06	0.0000E+00	0.0000E+00	1.5616E+06
13	216.48	-3.5988	0.0000	3.6046E+06	0.0000E+00	0.0000E+00	1.7098E+06
14	223.14	-4.2655	0.0000	3.7539E+06	0.0000E+00	0.0000E+00	1.8591E+06
15	229.81	-4.9321	0.0000	3.9042E+06	0.0000E+00	0.0000E+00	2.0094E+06
16	236.48	-5.5988	0.0000	4.0556E+06	0.0000E+00	0.0000E+00	2.1608E+06

### HEATING CURVE (CONTINUED)

MASS FLOW RATE	DENSITY	SPECIFIC GRAVITY	MOLECULAR WEIGHT
LB/HR	LB/FT3		

VAPOR	PHASE		
1	4.6747E+04	0.146	48.278
2	4.6747E+04	0.140	48.278
3	4.6747E+04	0.133	48.278
4	4.6747E+04	0.126	48.278
5	4.6747E+04	0.120	48.278
6	4.6747E+04	0.114	48.278
7	4.6747E+04	0.108	48.278
8	4.6747E+04	0.102	48.278
9	4.6747E+04	0.096	48.278

10	4.6747E+04	0.091	48.278
11	4.6747E+04	0.085	48.278
12	4.6747E+04	0.080	48.278
13	4.6747E+04	0.074	48.278
14	4.6747E+04	0.069	48.278
15	4.6747E+04	0.064	48.278
16	4.6747E+04	0.059	48.278

HEATING CURVE (CONTINUED)

VISCOSITY	THERMAL	CP	CV
CP	BTU/FT/HR/F	BTU/LBMOL/R	
-----			
VAPOR	PHASE		
1	0.9492E-02	0.0126	20.801 18.696
2	0.9598E-02	0.0129	20.965 18.867
3	0.9704E-02	0.0131	21.129 19.038
4	0.9814E-02	0.0134	21.292 19.209
5	0.9920E-02	0.0136	21.457 19.380
6	0.1002E-01	0.0139	21.622 19.551
7	0.1014E-01	0.0141	21.787 19.723
8	0.1024E-01	0.0144	21.953 19.894
9	0.1035E-01	0.0147	22.120 20.066
10	0.1046E-01	0.0149	22.286 20.237
11	0.1057E-01	0.0152	22.453 20.409
12	0.1068E-01	0.0155	22.620 20.581
13	0.1079E-01	0.0157	22.788 20.752
14	0.1089E-01	0.0160	22.955 20.924
15	0.1100E-01	0.0163	23.123 21.095
16	0.1112E-01	0.0166	23.290 21.267

PRESSURE, PSIG	BUBBLE POINT, F	DEW POINT, F	WATER DEW PT, F
-----			
4.4012	-196.88	136.46	76.779
-5.5988	-223.20	121.00	55.681
-----			

## Calculation Options: Condensate Recovery

CONDensate RECOvery = 4,-42

Sample output is shown below.

CONDENSATE PRODUCT RECOVERY SUMMARY

STREAM NUMBER 42

CONDENSATE RECOVERY

NITROGEN	1.47725 E-03
CO2	2.60193 E-02
METHANE	0.52137
ETHANE	0.31464
PROPANE	0.36588
I-BUTANE	0.22439
N-BUTANE	0.18067
I-PENTANE	0.13793
N-PENTANE	9.57027 E-02
N-HEXANE	0.27283
N-OCTANE	1.6359
TOTAL	3.7768
GALLONS/MSCF FEED	

## Calculation Options: Lost Work Analysis

A sample output for LOST work is shown below.

LOST WORK ANALYSIS SUMMARY

EQUIPMENT	USER	EXT. WORK	EXT. HEAT	EXCHANGE	LOST WORK
NUMBER	TYPE	NAME	BTU/HR	TEMP F	BTU/HR
-----					
1	HEAEXC	MKUP	-	-	4.144E+04
2	HEAEXC	HI-P	-	-	1.729E+05
3	VAL	DEAE	-	-	1.162E+06
4	PUM	BFW	-3.435E+05	-	3.177E+04
5	HEAEXC	PHT	-	-	5.315E+05
6	HEAEXC	ECON	-	1.903E+07 540.97	2.226E+06

# Chapter 8

7	DIV	BD	-	-	-	0.000E+00
8	HEAEXC	BOIL	-	9.769E+07	925.97	1.610E+07
9	DIV	PLAN	-	-	-	0.000E+00
10	EXP	STG1	5.345E+06	-	-	1.092E+06
11	DIV	EXT1	-	-	-	0.000E+00
12	EXP	STG2	6.017E+06	-	-	1.703E+06
13	DIV	EXT1	-	-	-	0.000E+00
14	EXP	STG3	1.742E+06	-	-	5.368E+05
15	MIX	COND	-	-	-	1.456E+04
16	HEAEXC	COND	-	-4.027E+07	70.33	8.880E+06
17	PUM	COND	-4.609E+03	-	-	365.
20	VAL	BDFL	-	-	-	1.135E+05
100	DIV	SET	-	-	-	0.000E+00
-----						-----
TOTAL						3.2609E+07

\*NOTE: IF LOST WORK IS NEGATIVE, REVIEW PARAMETERS FOR EQUIPMENT.

## AVAILABILITY FUNCTION SUMMARY

STREAM NO	AVAIL. FUNC. BTU/HR	STREAM NO	AVAIL. FUNC. BTU/HR
1	-3.00512E+06	90	2.79409E+06
10	-5.12535E+06	91	1.25121E+06
11	-2.99659E+06	95	1.00007E+06
12	-2.84326E+06	100	3.86831E+07
20	-3.87938E+06	110	1.54677E+07
21	-4.20560E+06	120	2.32015E+07
30	-7.28549E+05	121	1.67645E+07
40	-1.32373E+07	122	1.39704E+07
41	-1.29256E+07	123	6.25042E+06
42	-1.19142E+07	124	5.25035E+06
43	-5.31865E+06	125	2.97131E+06
44	-5.06547E+06	126	-1.24884E+06
50	1.25372E+06	127	-9.62003E+06
60	-2.53182E+05	128	-9.61578E+06
70	1.14878E+05	500	3.86692E+07
80	-4.81609E+05	900	-2.12023E+06
81	-5.31570E+05		

### DEFAULT OR SPECIFIED PARAMETERS:

AMBIENT TEMPERATURE: 77.03F  
 HEATING FLUID TEMPERATURE: 250.03F  
 COOLING FLUID TEMPERATURE: 70.33F  
 REFRIGERANT TEMPERATURE: -99.67F

LOST WORK CALCULATED BY METHOD OF NEVERS AND SEADER  
 REFERENCE: ENERGY, VOL.5, 757 (1980)

$$\text{LOST WORK} = \text{BIN} - \text{BOUT} + (1. - \text{TAMB} / \text{TEXCH}) * \text{Q} - \text{W}$$

WHERE BIN, BOUT: AVAILABILITY FUNCTION OF STREAMS  
 AVAILABILITY FUNCTION = ENTHALPY - TAMB\*ENTROPY  
 TAMB: AMBIENT TEMPERATURE  
 TEXCH: TEMPERATURE AT WHICH HEAT IS TRANSFERRED  
 Q: HEAT TRANSFERRED IN AND OUT FROM THE EQUIPMENT  
 W: EXTERNAL WORK





# Chapter 9: Print Options

Several other commands control the kind and amount of output which will be generated by a DESIGN II simulation. These are listed as *Print Options-General*. The print commands are divided into four categories:

- format control,
- standard output control,
- petroleum stream output control, and
- plot output control.

The DETAILED STREAM print will report the stream density, specific gravity, and the volumetric flow rate for each phase of a two phase stream.

## Print Options General

The following commands allow you to choose the kind and amount of output you receive from your simulation.

---

### Print Options: Format Control

---

The typical STREAM SUMMARY and DETAILED STREAM output shows 5 significant figures for each value printed, but the decimal points are not aligned. If you want the STREAM SUMMARY and DETAILED STREAM printed with decimals aligned, simply enter the DECimals for STReams command with a value for the number of digits which are to be printed after the decimal point. Maximum is 10. Due to space limitations between columns in the detailed stream summary section, any DEC STR value greater than 5 will use 5 in this section.

#### DECimals for STReams =

Enter a value for the number of digits to be printed after decimals in the stream summary print. Maximum value is 10. Default is 5 significant figures (decimals not aligned).

#### PRInt WIDe

Specify 132 column stream summaries. Use this command with the LINE module to get a break down of pressure drop due to acceleration for each segment.

The Stream Summary section will print seven streams per page, rather than four. Equipment module reports in the Equipment Summaries will also print seven unit operation reports per page. DISTillation and REFine column reports will continue to have a separate, detailed page for each unit as will the Heat Exchanger Rating results.

---

### Print Options: Standard Output Control

---

#### PRInt STReam =

Controls output printing of detailed stream summaries.

Only the stream numbers listed will have detailed stream summaries printed. If no detailed stream summary printout is desired, enter **NONE** after the equals sign. Default is all streams, if command is left out, unless you have one of the following specified in your input: REFine module, CRUde feed section or PETroleum STReam command.

**NOTE:** The following mixture properties are reported **only** in detailed stream summary:

**REID** vapor pressure (REI AST, REI CRU, REI PRO)  
**CO2 FREeze**  
**CRItical PRO**erties

**PRE**ssure **HYD**rate  
**TEM**perature **HYD**rate  
**CON**densate **REC**overy

#### PRInt UNIT STReam =

Controls print of feed and product streams before and after each call to a unit module.

#### PRInt FREquency =

Allows you to specify the number of iterations after which the STREAM SUMMARIES are printed during recycle loop calculations. PRInt FREquency = 2 is recommended; stream summaries will be printed after every second loop. If you use the following commands:

**MAX** loops = 5

#### PRInt FREquency = 4

you would obtain the summaries at the end of the calculations for the fourth iteration of the recycle loop. If the problem did not converge in five loops, you would also get the stream summaries at the end of the fifth iteration allowing you to compare iteration 4 with 5 to see if the problem is nearing convergence. Without the PRInt FREquency command, stream summaries will print after the last iteration. This command also controls rigorous column detailed prints (tray-by-tray sizing and plots) for any column within the recycle loop.

#### PRInt SWItch = 3

Enter this command to reduce the information printed for iterations of a recycle loop. This minimizes the output from a DESIGN II run.

## Chapter 9

---

### **PRInt SUMmaries =**

Enter the number of streams for which you want a report in the Stream Summary section of output. The streams will be printed in the order you enter them. Options are stream numbers, separated by commas, or NONE. Default is for all streams to print in ascending order.

The order of the streams in the PRI SUM command is the order in which they will appear in the stream summary.

---

### **Print Options: Stream Naming Command**

---

The stream names shown in the stream dialog are now transferred to DESIGN II using the NAM STR x command, where x is the stream number. The stream names appear in both the Stream Summary and Detailed Stream Print reports in the DESIGN II output file. The maximum length for the stream names is 24 characters (up to 14 characters will be printed in the stream summary table). The stream names are also transferred to Excel.

**NOTE:** Stream Name with apostrophes are not allowed. Example: C30's

---

### **Print Options: Ionic Stream Output Control**

---

For simulation using either EPSOURK or EDWARDK (ionic thermodynamic correlations), you may request a report detailing the ionic composition of each stream in the flowsheet. This information will print in the Stream Summary section of the output. The stream summary report and ionic stream reports will be merged (4 streams with regular data, 4 streams with ionic report, etc.)

### **PRInt IONic =**

Enter the stream numbers for which you want ionic compositions reported, separated by commas, or ALL. The default option is no report.

---

### **Print Options: Petroleum Stream Output Control**

---

For simulations having a CRUde feed section, the default detailed stream summary output will be a two-page report for each phase. The first page will report flows in lbmoles per hour, pounds per hour and barrels per day (metric-kgmol/hr, kg/hr, normal cubic meters per hour) for each component. The second page will include TBP, ASTM D-86 distillation curves, gravity curves, and other stream properties. The vapor phase, if any, is reported first, then the liquid phase.

### **PETroleum STReams =**

Controls output printing of the two page report for streams which includes distillation curves. Options are **ALL**, stream numbers, or **NONE**. Default is all streams if command is left out (and CRUde feed section is used).

**NOTE 1:** You can get either type of detailed stream report for any stream. If your simulation does not include a CRUde feed section, water (id number 62) **must** be first in the COMponent list and all other components must be entered in ascending boiling point order. In simulations with a CRUde feed section may enter either or both the PRI STR and PET STR commands. Each command should list the stream numbers for which that format report is desired. No report will be printed for a stream which is not listed on either command.

**NOTE 2:** If you do not request any format when CRUde section and/or REFINe column is present, both stream formats (regular and petroleum) for all streams in the flowsheet will be printed.

If you want regular detailed stream summary for few streams and petroleum stream formats for certain streams in the presence of REFINe or CRUde section, please enter the following commands:

**PRInt STReams = X, Y**

**PETroleum STReams = A, B, C,**

If you want both formats (regular and petroleum) for the requested streams plus regular detailed stream summary for the remainder of the streams in the flowsheet when REFINe or CRUde section is present, please enter the following commands:

**PETroleum STReams = A, B, C,**

If you want both formats (regular and petroleum) for the requested streams plus petroleum stream summary for the remainder of the streams in the flowsheet when REFINe or CRUde section is present, please enter the following commands:

**PRInt STReams = A, B, C,**

Instead of a list of stream numbers, you may enter the words "ALL" or "NONE" on either command. If you **do not** want regular stream summary and **NEED** only the petroleum stream format for certain streams, please enter the following commands:

**PRInt STReam = NONE**

**PETroleum STReam = X, Y, Z,**

If you **do not** want petroleum stream summary and **NEED** only the regular detailed stream format for certain streams, please enter the following commands:

**PRInt STReam = X,Y,Z**

**PETroleum STReam = NONE,**

If you want regular detailed stream summary for all streams and do not want petroleum stream formats for any stream in the presence of REFINe or CRUde section, please enter the following commands:

**PRInt STReams = ALL**

**PETroleum STReams = NONE**



If you do not want any detailed reports at all, use the following commands:

**PRInt STReams = NONE**  
**PETroleum STReams = NONE**

If your simulation does not include a CRUde feed section, or you want to limit the streams for which this report is generated, simply enter the PRI STR commands. Options are ALL, NONE or individual stream numbers (in ascending order). If you do not want detailed stream reports, enter:

**PRInt STReams = NONE**  
*or*  
**PETroleum STReams = 1, 10, 15**

**API ENThalpy**

Enter this command to get API ENThalpies printed with the petroleum stream output using a -200 F, saturated liquid base in addition to the enthalpies normally reported using base conditions of ideal gas at 32F, 14.696 PSIA. This option should only be used with the API and API MOD enthalpy options.

**ASME ENThalpy**

Enter this command to get enthalpies generated for saturated liquid at 32 F enthalpy / entropy base conditions.

**NOTES:**

1. If both the **API ENThalpy** and **ASME ENThalpy** commands are present then all components except water use the 200 F saturated liquid base conditions. Water uses the 32 F saturated liquid base condition. Also, added a warning message, if the latent heat for a component is zero as: **WARNING: The calculated latent heat for component id 46 is zero at 259.67 R.** Please choose another saturated liquid enthalpy base that is below the critical temperature for this component. Or, revert to the ideal gas enthalpy base.
2. The mixed amine thermodynamic method has not been modified for these options

**PROduct IBP =**

Enter this command to change the initial volume percent in the distillation curves. Default is 2 volume percent.

**PROduct EP =**

Enter this command to change the volume percent for the end point of the distillation curves. Default is 98.

---

**Print Options: Plot Output Control**

---

You can request one or more plots of one or two variables against length for one or more LINE modules. Several different PLOt commands may be used in the same run. Each PLOt command will generate a separate plot.

**PLOT** variable 1 against Length for line = i1, i2, i3,...

*or*

**PLOT** variable 1 **AND** variable 2 against length for line = i1, i2, i3,...

Variable 1 and variable 2 are keywords from the list below. The i1, i2, i3, etc., are the equipment numbers of LINE modules connected in series on the flowsheet. The length used in the plot is the cumulative length from the start of the first LINE to the end of the last LINE.

<b>DEL</b> ta p <b>ELEV</b> ation	<b>HOL</b> dup	<b>TEM</b> perature
<b>DEL</b> ta p <b>FR</b> iction	<b>PRE</b> ssure	<b>VEL</b> ocity
<b>ELEV</b> ation		

**NOTE:** The PLOt command belongs in the GENeral section.

Several equipment modules have plots which print automatically: DIStillation columns, HEAt EXChanger, REFIne columns, and SHORtcut fractionators.

These plots are suppressed automatically for all but the final iteration of recycle loop calculations. This will also suppress plots for HEAtInG CURve, COOLing CURve and PLOT LINES.

**PLOT OFF**

Enter this command to delete default plots for HEAt EXChanger, DIStillation column, REFIne column, SHORtcut fractionator, and HEAtInG or COOLing CURves.

**Print Options Command Summary**

**Format Control**

**DEC**imals of **STR**eams =

**Standard Output Control**

**PR**Int **STR**eam =  
**PR**Int **UN**It **STR**eam =  
**PR**Int **FR**equency =

**Petroleum Stream Output Control**

**PET**roleum **STR**eams =  
**API EN**Thalpy

**PLOT Commands**

**PLOT** variable 1 against length for line = i1, i2, i3, ..  
**PLOT** variable 1 **AND** variable 2 against length for  
line = i1, i2, i3, ...  
**PLOT OFF**

# Chapter 9

PROduct IBP =  
PROduct EP =

## Print Options Step by Step

### Print Options STEP 1

**Format control. Select any of the GENERAL section print options listed below:**

Number of digits to be printed after decimals in the stream summary (maximum value is 10; default is 5)	<b>DEC STR =</b>
Standard Output Control	
Print detailed stream summaries for streams listed in ascending order or <b>NONE</b> after the equals sign for no detailed stream summary (default is all streams)	<b>PRI STR =</b>
Controls print of feed and product streams before and after each call to a unit module.	<b>PRI UNI STR =</b>
Print STREAM SUMMARIES after "n" iterations for recycle loops	<b>PRI FRE = n</b>
Petroleum Stream Output Control (MUST have a CRUde feed section)	
Controls output printing of the two page report for streams which includes distillation curves (options are <b>ALL</b> , stream numbers, or <b>NONE</b> ; default is all streams)	<b>PET STR =</b>
Print API ENThalpies with the petroleum stream output using a -200 F, saturated liquid base in addition to the enthalpies normally reported using base conditions of ideal gas at 32 F, 14.696 PSIA (this option should only be used with the API and API MOD enthalpy options)	<b>API ENT</b>
Change the initial volume percent in the distillation curves (default is 2 volume percent)	<b>PRO IBP =</b>
Change the volume percent for the end point of the distillation curves (default is 98)	<b>PRO EP =</b>

### Print Options STEP 2

**Plot output control, select a PLOT command.**

- **PLOT** variable 1 against length for line = i1, i2, i3, ..
- **PLOT** variable 1 **AND** variable 2 against length for line = i1, i2, i3, ..

Variable 1 and variable 2 are keywords from the list below. The i1, i2, i3, etc., are the equipment numbers of LINE modules connected in series on the flowsheet. The length used in the plot is the cumulative length from the start of the first LINE to the end of the last LINE.

<b>DEL</b> ta p <b>E</b> LEvation	<b>HOL</b> dup	<b>TEM</b> perature
<b>DEL</b> ta p <b>FRI</b> ction	<b>PRE</b> ssure	<b>VEL</b> ocity
<b>E</b> LEvation		

- The PLOt command belongs in the GENERAL section.
- Delete default plots for HEAt EXChanger, DIStillation column, REFine column, SHORtcut fractionator and HEAting or COOLing CURves **PLOT OFF**

## Print Options Examples

### Print Options: Stream Summary

Regular output is shown here.

STREAM SUMMARY				
STREAM NUMBER	1	2	3	4
STREAM NAME	Strm 1	Strm 2	Strm 3	Strm 4
EQUIP CONXION	FEED-X-1	X-1 -F-2	F-2 -E-3	E-3 -F-4
	( 0)-( 1)	( 1)-( 2)	( 2)-( 3)	( 3)-( 4)
VAPOR FRACTION	0.98818	0.82510	1.0000	0.90408
TEMPERATURE F	90.000	-35.000	-35.000	-129.49
PRESSURE PSIA	994.70	984.70	984.70	275.00
ENTHALPY BTU/HR	-0.16524E+07	-0.17440E+08	-0.98039E+07	-0.12735E+08
V Cp BTU/LBMOL/R	12.974	18.359	18.359	10.357
V Cv BTU/LBMOL/R	8.4817	7.4686	7.4691	6.0966
L Cp BTU/LBMOL/R	32.263	21.651		17.658
V DEN LB/FT3	3.9509	5.8772	5.8772	1.5752
L DEN LB/FT3	31.589	27.807		29.424
L S.G. (60F) STP	0.55130	0.43451		0.37643
V VIS CP	0.13517E-01	0.12507E-01	0.12507E-01	0.78150E-02
L VIS CP	0.13427	0.97874E-01		0.11918
V THC BTU/FT/HR/F	0.24073E-01	0.22708E-01	0.22708E-01	0.14214E-01
L THC BTU/FT/HR/F	0.62751E-01	0.68921E-01		0.84454E-01
V MMSCF/DAY STP	63.620	53.121	53.121	48.026
L GAL/MIN STP	15.654	180.52		78.069
TOTAL MOLE WEIGHT	19.911	19.911	17.406	17.406

L-LIQUID PHASE (EXCLUDING IMMISCIBLE WATER), V-VAPOR PHASE  
 Cp,Cv-HEAT CAPACITY, DEN-DENSITY, VIS-VISCOSITY, THC-THERMAL CONDUCTIVITY

FLOW RATES		LBMOL/HR			
METHANE		6100.0	6100.0	5408.9	5408.9
ETHANE		500.00	500.00	320.80	320.80
PROPANE		200.00	200.00	76.681	76.681
N-BUTANE		100.00	100.00	17.849	17.849
N-PENTANE		100.00	100.00	7.2844	7.2844
N-HEXANE		70.000	70.000	2.0071	2.0071
TOTAL		7070.0	7070.0	5833.5	5833.5
TOTAL	LB/HR	0.14077E+06	0.14077E+06	0.10154E+06	0.10154E+06

**Print Options: ASTM 86 Distillation**

Portions of PETroleum STream output are shown below. Flash point and several other properties of interest to refinery calculations are automatically included in this report.

STREAM NUMBER		CONNECTING		( 0) FEED		
NAME: Strm 1		TO ( 100) VAC				
MESO K-VALUES	APIM ENTHALPY	STD	DENSITY	FLOW RATES /HR		
COMPONENT NAME	TOTAL LBMOL	LIQUID LBMOL	VAPOR LBMOL	TOTAL LB	TOTAL MOL PCT	KVALUE
WATER	0.	0.	0.	0.	0.	
382 F ABP	3.98658	3.98658	0.	543.678	1.4873	
407 F ABP	3.79606	3.79606	0.	549.027	1.4163	
432 F ABP	4.11668	4.11668	0.	630.737	1.5359	
457 F ABP	4.42249	4.42249	0.	717.020	1.6500	
482 F ABP	4.22162	4.22162	0.	723.483	1.5750	
507 F ABP	5.86127	5.86127	0.	1060.59	2.1868	
532 F ABP	7.02331	7.02331	0.	1340.38	2.6203	
557 F ABP	6.72197	6.72197	0.	1351.56	2.5079	
582 F ABP	10.3037	10.3037	0.	2180.24	3.8442	
607 F ABP	10.4661	10.4661	0.	2328.05	3.9047	
632 F ABP	10.0443	10.0443	0.	2346.11	3.7474	
657 F ABP	16.1199	16.1199	0.	3949.39	6.0141	
682 F ABP	18.3208	18.3208	0.	4703.00	6.8352	
707 F ABP	18.0655	18.0655	0.	4853.61	6.7400	
744 F ABP	36.0646	36.0646	0.	10353.3	13.455	
794 F ABP	33.0652	33.0652	0.	10329.3	12.336	
844 F ABP	25.6030	25.6030	0.	8665.25	9.5521	
894 F ABP	16.6634	16.6634	0.	6083.22	6.2169	
944 F ABP	11.2578	11.2578	0.	4413.61	4.2001	
994 F ABP	8.07701	8.07701	0.	3385.69	3.0134	
1069 F ABP	7.20818	7.20818	0.	3313.02	2.6893	
1169 F ABP	2.58927	2.58927	0.	1325.03	0.96602	
1269 F ABP	1.98258	1.98258	0.	1109.89	0.73967	
1369 F ABP	1.55743	1.55743	0.	937.159	0.58106	
1435 F ABP	0.495863	0.495863	0.	309.993	0.18500	
TOTAL	268.035	268.035	0.	77502.3	100.000	
TOTAL LB	77502.3	77502.3	0.			

STREAM NUMBER 1  
 TEMPERATURE DEG F 650.00  
 PRESSURE PSIA 95.000  
 ENTHALPY BTU/HR 1.05326E+07  
 VAPOR FRACTION 0.00000E+00

PROPERTIES	TOTAL	LIQUID
FLOWRATE LBMOL/HR	268.0346	268.0346
MOLECULAR WT.	289.1503	289.1503
ENTHALPY BTU/LBMOLE	39295.7266	39295.7266
ENTROPY BTU/LBMO/R	64.8367	64.8367
CP BTU/LBMOL/R		176.6245
CV BTU/LBMOL/R		166.6915
DENSITY LB/FT3		52.7472
Z-FACTOR		0.043738
FLOWRATE GAL/MIN T-P		183.1992
S.G. (TS/60) GPA STP		1.0624
VISCOSITY CP		0.492306
TH.COND BTU/FT/HR/F		0.038624
SURFACE TENSION DYNE/CM		16.0086

STREAM NUMBER 1 MESO K-VALUES APIM ENTHALPY

# Chapter 9

NAME: Strm 1  
CONNECTING FEED-VAC  
0 - 100

## LIQUID PORTION OF STREAM

		LBMOL/HR	LB/HR	BBL/DAY
1	WATER	0.00000E+00	0.00000E+00	0.00000E+00
2	382 F ABP	3.9866	543.68	39.835
3	407 F ABP	3.7961	549.03	39.836
4	432 F ABP	4.1167	630.74	45.333
5	457 F ABP	4.4225	717.02	51.061
6	482 F ABP	4.2216	723.48	51.061
7	507 F ABP	5.8613	1060.6	74.202
8	532 F ABP	7.0233	1340.4	92.981
9	557 F ABP	6.7220	1351.6	92.981
10	582 F ABP	10.304	2180.2	148.78
11	607 F ABP	10.466	2328.1	157.62
12	632 F ABP	10.044	2346.1	157.62
13	657 F ABP	16.120	3949.4	263.33
14	682 F ABP	18.321	4703.0	311.27
15	707 F ABP	18.066	4853.6	318.93
16	744 F ABP	36.065	10353.	673.17
17	794 F ABP	33.065	10329.	662.56
18	844 F ABP	25.603	8665.3	548.63
19	894 F ABP	16.663	6083.2	380.35
20	944 F ABP	11.258	4413.6	272.64
21	994 F ABP	8.0770	3385.7	206.72
22	1069 F ABP	7.2082	3313.0	198.92
23	1169 F ABP	2.5893	1325.0	77.893
24	1269 F ABP	1.9826	1109.9	63.963
25	1369 F ABP	1.5574	937.16	53.005
26	1435 F ABP	0.49586	309.99	17.326
		268.03	77502.	5000.0

TEMP = 650.00 F  
PRES = 95.000 PSIA  
ENTH = 0.10533E+08 BTU/HR  
ENTH = 0.24250E+08 BTU/HR (API)  
WT = 289.15

(WATER-FREE BASIS FOR CUMULATIVE VOLUME PERCENTS AND DISTILLATION CURVES)

### LABORATORY DISTILLATION

NO	COMPONENTS	VOL PCT	CUM VOL	VOL	API	DEG F TBP	D 86 ASTM
1	WATER	0.000	0.00	2.	17.0	430.13	469.29 *
2	382 F ABP	0.797	0.80	5.	13.2	500.82	525.72 *
3	407 F ABP	0.797	1.59	10.	10.0	568.74	579.93
4	432 F ABP	0.907	2.50	20.	6.6	646.65	645.58
5	457 F ABP	1.021	3.52	30.	4.7	691.79	683.63
6	482 F ABP	1.021	4.54	40.	3.3	730.28	712.51
7	507 F ABP	1.484	6.03	50.	1.9	767.85	740.69
8	532 F ABP	1.860	7.89	60.	0.5	806.44	772.48
9	557 F ABP	1.860	9.75	70.	-0.9	848.86	807.42
10	582 F ABP	2.976	12.72	80.	-2.8	906.35	862.60
11	607 F ABP	3.152	15.87	90.	-5.6	999.35	951.85
12	632 F ABP	3.152	19.03	95.	-8.7	1113.54	1001.96 *
13	657 F ABP	5.267	24.29	98.	-12.6	1272.96	1071.92 *
14	682 F ABP	6.225	30.52	* = AN EXTRAPOLATIVE VALUE			
15	707 F ABP	6.379	36.90				
16	744 F ABP	13.463	50.36				
17	794 F ABP	13.251	63.61				
18	844 F ABP	10.972	74.58				
19	894 F ABP	7.607	82.19				
20	944 F ABP	5.453	87.64				
21	994 F ABP	4.134	91.78				
22	1069 F ABP	3.978	95.76				
23	1169 F ABP	1.558	97.31				
24	1269 F ABP	1.279	98.59				
25	1369 F ABP	1.060	99.65				
26	1435 F ABP	0.347	100.00				

### LIQUID PROPERTIES

TEMPERATURE F = 650.00  
PRES. PSIA = 95.000  
ENTH. BTU/HR = 0.10533E+08  
MOLECULAR WEIGHT = 289.15  
Z-FACTOR T,P = 0.43733E-01  
LB/FT3 T,P = 52.747  
US GPM T,P = 183.19  
GAL/MOLE STP = 32.645  
S.G. STP = 1.0623  
BBSPD STP = 5000.0

```
DEG API STP      = 1.7000
LB/GAL STP      = 8.8574
LB/BBL STP      = 372.01
UOPK           = 10.092
FLASH PT EM F   = 267.98
MABP DEG F     = 723.67
VABP DEG F     = 752.70
COND. BTU/FT/H  = 0.38624E-01
SP HEAT BTU/LB/F = 0.61084
S.T. DYNES/CM   = 16.009
VS. CP         T = 0.49231
      CP      100F = 175.29
      CP      210F = 11.345
++ STP = 60 DEG F, 14.7 PSIA
* = AN EXTRAPOLATIVE VALUE
```

---

## Print Options: Use of the PLOT commands

---

For an example of the PLOT command, see *Line: Intermediate Compression and Junction* problem in the LINE module.



# Chapter 10: Recycle Loops

There are several commands you can use for recycle loop problems which allow you to:

- Review the sequence of equipment calculations (which is automatically generated by DESIGN II) to easily determine the streams for which you will need to provide initial guesses for flowrates, temperature and pressure.
- Provide initial guesses for flowrates, temperature and pressure for one or more recycle streams.
- Limit the number of iterations for the recycle loop.
- Loosen or tighten the tolerance for heat and material balance convergence.
- Direct the sequence of calculations.
- Stop calculations at a specific equipment module. Control the volume of output produced.

Additionally, case studies can be performed on individual equipment or on flowsheets with recycles.

## Recycle Loops Initial Guesses

**FLO** (Q units/t units) j =  
and

**TP** (T units, P units) j =

Enter a FLO and TP command for each internal stream for which you are providing initial guesses for the recycle calculation (see SPECIFYING FEEDS Section for details).

If either flowrate (and compositions) or temperature and pressure of a recycle stream are the same as (or very close to) a feed stream, you can use either of the following commands:

FLO x = FLO y

TP x = TP y

where "x" represents the recycle stream number and "y" represents the feed stream you want to copy.

## Recycle Loops Calculation Options

Any simulation problem is converged when all differences between the present iteration and the previous iteration are within the specified CONvergence TOLerance. Convergence tolerance determines the robust closure on mass and energy balances on the process. All the enthalpies, temperatures, and component flowrates are checked in every stream. The default value is 0.001, which corresponds to 0.1%.

For initial simulation runs or recycle estimates, consideration should be given to choose a convergence tolerance between 0.005 (.5% error) and 0.01 (1% error). Do not use a tolerance greater than 0.1 or 10%, since too great a tolerance can cause inconsistencies in equipment convergence, resulting in nonconvergence of the process.

SOLUTION HAS BEEN REACHED message indicates that the recycle loops have converged to the specified tolerance AND all the equipment modules in the process simulation have achieved convergence corresponding to their individual specifications.

---

## Recycle Loops: Wegstein

---

Wegstein technique is a convergence method where an acceleration judgment is used on individual recycle stream behavior. The Wegstein convergence acceleration begins after the third iteration of the process loop. Individual component flowrates for streams entered on the RECYCLE STReam command will be increased or decreased by a Wegstein factor as calculated from previous iterations. The temperature of a stream can be accelerated in convergence by entering the stream number on a CONvergence on TEMperature command.

The CON TEM command is used only when temperature, rather than component flowrates, is changing significantly during convergence.

The acceleration factor Q is printed for the component flowrates or temperature of the designated stream(s) after the third iteration.

- If Q is a negative number, the Wegstein technique is accelerating convergence.
- If Q is zero, direct substitution will be used.
- If Q is between zero and .5, your process is oscillating but should converge. The Wegstein technique will damp the oscillations. If Q is greater than .5, your process is oscillating in a divergent manner and may not converge, although the Wegstein technique will damp the oscillations.

Non-convergence occurs when the process is unstable. Additional control for process variables is needed. If the Wegstein Q remains positive and greater than .5 for several loops for one or more components in any stream, a careful review of your flowsheet and output may uncover the problem which is causing non-convergence. Some typical situations that can cause oscillatory divergence are:

- single component stream changing phase

## Chapter 10

---

- unstable temperature where a flash is occurring
- material is trapped or building up very slowly in the recycle loop

**RECycle STReams** = j, k, ...

Enter stream number(s) for the minimum recycle streams for which component flowrates are to be accelerated using the Wegstein or Simultaneous Convergence techniques.

**CONverge on TEMperature** = j, ...

Enter stream number(s) for accelerated convergence on the temperature. Use only when temperature, not component flowrates, is changing significantly during convergence.

**CONvergence TOLerance** =

Enter the heat and material balance convergence tolerance you want the program to achieve. Default is 0.001(.1%).

**NOTE:** If you are choosing your own RECycle STReams (or) via Recycle Loops: Specified Sequence, consider entering FLOWrates and TP for a feed to a phase separation module (FLA or VAL) rather than one or both of the products from the module. This minimizes the number of recycle streams, and convergence tends to be faster particularly if the flash temperature changes from one loop to the next.

---

### Recycle Loops: Direct Substitution

---

Direct Substitution is a convergence method in which current values of temperature, pressure, and flows are used for subsequent iterations until the convergence tolerance is satisfied.

**DIRect SUBstitution**

Specifies use of direct substitution as the convergence method.

**DIRect SUBstitution** = n

Specifies use of direct substitution for first "n" loops (to be used along with SIM CON technique. Default is first loop)

**CONvergence TOLerance** =

Enter the heat and material balance convergence tolerance you want the program to achieve. Default is 0.001(.1%).

There are situations, however, where specifying the recycle sequence may be helpful. These situations normally involve CONTROLLER modules which interfere with the logical order of calculations or situations where intermediate stream properties are known. See Controller Section for more details.

A REC SEQ command may be used to specify the order of equipment even if there is no recycle. Please see Recycle Loops: Specified Sequence for more details. A REC SEQ 2 command may be useful in situations where there is a recycle loop and also equipment modules which are to be calculated after the loop.

**RECycle SEQuence** = k, ...

Enter equipment numbers (from flowsheet) in the order in which you wish them to be calculated. Rarely required, since DESIGN II automatically determines the logical order. This command can be used to replace the Wegstein convergence technique with direct substitution if no REC STR command is entered.

**NOTE1:** SIM CON and DIR SUB are disabled if the run has an OPTIMIZATION section. The program automatically determines the optimum order in which the equipment in a recycle loop should be calculated and reports the stream numbers for the minimum streams that need to be guessed to solve the problem. By using a CHECK INPUT command, you can have this information reported for evaluation before the complete run is made. The RECycle STReams command is used to enter the stream numbers for which you will enter guesses (TP and FLOW commands). The component flows and enthalpies in these streams will be accelerated individually using the Wegstein (default) convergence technique. If the temperature (not component flowrates) is the only recycle stream property changing with each iteration, the CONvergence on TEMperature command will accelerate convergence, again using the Wegstein technique. The RECycle STReams command should never contain more streams than the minimum required by the program.

**NOTE2:** If you want Wegstein or SIM CON acceleration of recycle streams when you are specifying REC SEQ, be sure to enter a RECycle STReams command. Otherwise, the recycle calculation will be performed using direct substitution only.

---

### Recycle Loops: Simultaneous Convergence

---

The SIMultaneous CONvergence technique should be used primarily for linked columns and heat exchanger networks with SIM or TEM APP specifications. Acceleration judgment for material balance (and temperature) convergence is made based on simultaneous evaluation of all recycle streams. This differs from the Wegstein technique where acceleration judgment is based on individual recycle stream behavior. The direct substitution technique does not perform convergence acceleration.

**SIMultaneous CONvergence**

Specifies use of a Newton-Raphson convergence technique. Used primarily for linked columns.

The CON TEM command is used only when temperature, rather than component flowrates, is changing significantly during convergence.

**RECycle STReams** = j, k, ...

Enter stream number(s) for the minimum recycle streams for which component flowrates are to be accelerated using the Wegstein or Simultaneous Convergence techniques.



**CON**verge on **TEM**perature = j, ...

Enter stream number(s) for accelerated convergence on the temperature. Use only when temperature, not component flowrates, is changing significantly during convergence.

**SIM**ultaneous **CON**vergence **TEM**perature = k, ...

Enter stream numbers to be used as variables in the Newton-Raphson convergence calculation. This differs from **CON TEM** in that stream temperatures are **added** to the convergence calculations.

**NOTE 1:** **SIM CON** and **DIR SUB** are disabled if the run has an **OPTIM**ization section. The program automatically determines the optimum order in which the equipment in a recycle loop should be calculated and reports the stream numbers for the minimum streams that need to be guessed to solve the problem. By using a **CHECk INP**ut command, you can have this information reported for evaluation before the complete run is made. The **RECYcle STR**eams command is used to enter the stream numbers for which you will enter guesses (**TP** and **FLOW** commands). The component flows and enthalpies in these streams will be accelerated individually using the Wegstein (default) convergence technique. If the temperature (not component flowrates) is the only recycle stream property changing with each iteration, the **CON**vergence on **TEM**perature command will accelerate convergence, again using the Wegstein technique. The **RECYcle STR**eams command should never contain more streams than the minimum required by the program.

**NOTE 2:** If you are choosing your own **RECYcle STR**eams (or) via **Recycle Loops: Specified Sequence**, consider entering **FLOW**rates and **TP** for a feed to a phase separation module (**FLA** or **VAL**) rather than one or both of the products from the module. This minimizes the number of recycle streams, and convergence tends to be faster particularly if the flash temperature changes from one loop to the next.

**NOTE 3:** **SIM CON TEM** is disabled if the run has an **OPTIM**ization section.

---

## Recycle Loops: Specified Sequence

---

The **CAL**culati**ON** **SEQ**uence command will determine automatically the equipment modules which are involved in a recycle loop and will only recalculate those in the loop. The remainder of the equipment will be calculated once. Alternatively you can use a **RECYcle SEQ**uence command to specify your own recycle sequence, but all equipment modules to be calculated must be included whether they are in the process loop or not. In general, you are much better off allowing the program to determine the order.

There are situations, however, where specifying the recycle sequence may be helpful. These situations normally involve **CON**Troller modules which interfere with the logical order of calculations or situations where intermediate stream properties are known. See **Controller** Section for more details.

A **REC SEQ** command may be used to specify the order of equipment even if there is no recycle. A **REC SEQ 2** command may be useful in situations where there is a recycle loop and also equipment modules which are to be calculated after the loop.

If the **REC SEQ 2** command does not contain a recycle calculation (or controller), use the **STOP** command to prevent these equipment modules from being calculated twice. The value entered for the **STO** command should be the last equipment number on the **REC SEQ 2** command.

**CAL**culati**ON** **SEQ**uence = k, ...

Enter all equipment module numbers, separated by commas, in the order in which you wish them calculated. This command is available for Wegstein and **SIM**ultaneous **CON**vergence options.

**RECYcle SEQ**uence = k, ...

Enter equipment numbers (from flowsheet) in the order in which you wish them to be calculated. Rarely required, since **DESIGN II** automatically determines the logical order. This command can be used to replace the Wegstein convergence technique with direct substitution if no **REC STR** command is entered.

**RECYcle SEQ**uence 2 = k, ...

Use this command with **REC SEQ** to specify equipment calculation order when you have two separate recycle loops. Rarely required, since **DESIGN II** automatically determines the logical order.

**Example:**

**RECYcle SEQ**uence 2 = 7, 8, 9, 10,

**STOP** = 10,

**NOTE:** If you want Wegstein or **SIM CON** acceleration of recycle streams when you are specifying **REC SEQ**, be sure to enter a **RECYcle STR**eams command. Otherwise, the recycle calculation will be performed using **DIR**ect **SUB**stitution only.

A **ONE LOOP** general section command may be used for a recycle that allows entire flowsheet to be calculated in a single recycle loop that have potentially isolated tail end unit modules that can be added into the single loop. This is most applicable when:

1. There is a Mass Balance unit module in the loop and it needs product stream information that is outside the recycle loop.

## Chapter 10

2. There is Inline Fortran or Controller module in the recycle loop that needs information from unit modules / streams outside the loop.
3. There are internal streams outside the recycle loop that need to be calculated along with equipments inside the loop.

### ONE LOOP

Use this command to include all modules in the entire flowsheet to be calculated in a single recycle loop.

**Note:** This can cause large flowsheets with complex multi-level recycles not to converge or take an excessive time to converge. In these cases, it is recommended not to use this command but instead use the above two **CAL SEQ** and **REC SEQ** commands.

---

### Recycle Loops: Case Study

---

Case studies can be setup easily using Inline FORTRAN. For case studies with more than one equipment, the calculation order can be determined using the default calculation sequence analysis or can be specified directly using CAL SEQ or REC SEQ, REC SEQ 2. If you choose the REC SEQ commands you must specify REC STR. Please see Recycle Loops: Specified Sequence

**REPEAT** = j, ...

Enter number of case study trials.

Alternatively, use the Case Study flowsheet option.

---

### Recycle Loops: Control

---

The STOp command is used to specify an equipment number after which calculations will stop. It can be used to slowly work through a complicated flowsheet one step at a time. Also the STOp command can be used like the CHEck INPut command. The STOp command would be particularly useful when there are some equipment modules that could be calculated before the recycle is reached. By calculating these front-end equipments, information for recycle stream guesses might be obtained.

**STOp** after module =

Enter the equipment number after which you want calculations to stop so you can review calculation progress.

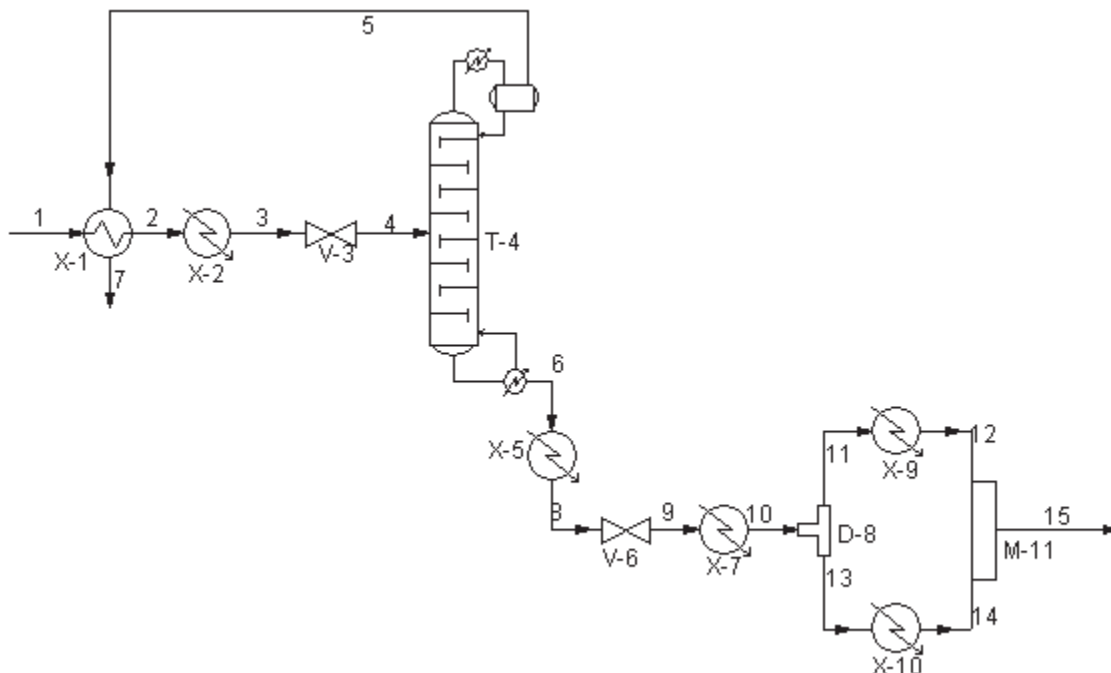
**PRInt FRE**quency =

Controls output printing of stream summaries during calculation loops: 2 is recommended (stream summaries will be printed after every second loop). This command also controls rigorous column detailed prints (tray-by-tray sizing, plots and K-values) for any column within the recycle loop.

---

### Recycle Loops: Example

---



The following recycle commands could be used:

**RECYCLE STR**eams = 4,

**RECYCLE SE**quence = 4, 1, 2, 3

**RECYCLE SE**quence 2 = 5, 6, 7, 8, 9, 10, 11

**MAX** loops = 5

The program will recognize that only equipment modules 1 through 4 are in a recycle loop, and will calculate them until convergence is reached (or iteration loop count reaches 5). Then equipment modules 5 through 11 will be calculated as the second recycle sequence.

Using the CALculation SEQuence command solves the same problem also in different equipment sequence order.

**REC STR** =4

**CAL SEQ** = 4, 1, 2, 3, 5, 6, 7, 8, 9, 10, 11

**MAX** = 5

The equipment calculated in the order 4, 1, 2, 3 will iterate until convergence, which may take three or four loops. The equipment calculated in the order 5, 6, 7, 8, 9, 10, 11 will be solved as a separate loop and will stop after calculating equipment 11. The alternative, if you must specify the equipment order, would be to code all equipments in one big loop, which may lead to additional iterations to solve.

**RECYCLE STR**eams = 4

**RECYCLE SE**quence = 4, 1, 2, 3, 5, 6, 7, 8, 9, 10, 11

**MAX** loops = 5

**NOTE:** The above commands are not normally required and we recommend users to allow simulator's automatic sequence analysis to converge the problem. In instances where nested loops or convergence difficulty using simulator's sequence are identified, it is up to the users to determine which set of equipment modules form the two recycle loops to facilitate closure of all loops.

## Recycle Loops Print Options

### **MAXimum loops =**

Use this command to limit the number of calculation loops the program will make seeking convergence; 10 is recommended. Default is 1.

The CHEck INPut command is recommended for the first run to avoid wasting time and money running a simulation with incorrect input data. For a detailed description of the information you would get with this command, see FLOWSHEET Section.

### **CHEck INPut**

This command is highly recommended for your initial run. No equipment calculations will be performed. The printout allows you to review input data and equipment calculation order. It also indicates the streams for which DESIGN II needs additional information to effectively calculate the recycle loop. Do **not** include a STOP command with the CHEck INPut command.

You can limit the amount of output produced during recycle calculations. Or you can request additional output to aid in analysis of composition or temperature changes from iteration to iteration.

### **PRInt FRE**quency

Enter a value for printing stream summaries during recycle loop calculations; stream summaries will be printed after every nth loop, where n is the value you entered. Default is no additional stream summary print.

### **PRInt SWItch**

Enter this command if you want to minimize the value of output generated during recycle loop calculation. Most of the information which would normally appear in the NOW CALLING section of output will be suppressed. Column convergence (final norm) will still print for DISTillation and REFine columns.

## Recycle Loops Reverse Calculation

Reverse Calculation is supported for very few modules at this time. They are flash, line, mixer, depressurizer and compressor. Product streams must be specified.

### **REVerse CAL**culatation

Specifies use of a reverse calculation of unit modules.

### **REVerse calculation MAX**imum iterations =

Enter reverse calculation unit module maximum iterations. Default is 1000.

### **REVerse calculation TOL**erance =

Enter the reverse calculation unit module tolerance. Default is 1 E-07.

### **NOTES:**

1. The procedure just reverses the current unit module calculation order. There is a unit module iterator that can iterate a single unit module to a given pressure error and enthalpy error with a maximum iteration count. The new keyword to trigger the reverse calc is: REVerse CALculatation. The new keywords to control the iterator are: REVerse TOLerance = 1.0e-7 (default) and REVerse MAXimum iterations = 1000 (default).
2. The unit modules to be reverse calculated must only have one inlet stream unless the unit module is the mixer. The mixer unit module has new commands to split the flow from the outlet stream into two or more inlet streams: FLO

## Chapter 10

(FRA) = inlet #1, inlet #2, ... or FLO (quantity/time) = inlet #1, inlet #2, ... You do not need to specify the last inlet stream fraction or flowrate as all of the remaining flow will be put into that stream. The flash unit module does not need to be iterated as it becomes a simple mixer of its outlet streams.

- The compressor, pump and expander unit modules have a new command for specifying the inlet pressure is to be for the calculation: PREssure INLet (pressure) = number. The inlet stream temperature will be automatically calculated based on inlet stream pressure and the outlet stream conditions.

### Recycle Loops Command Summary

#### Initial Guesses

**FLOW** (Q units/t units) j =  
**TP** (T units, P units) =

#### Calculation and Print Options

**MAX**imum loops =  
**CHE**ck **INP**ut  
**RECY**cle **STR**eams = j, k, ..  
**SIM**ultaneous **CON**vergence  
**DIR**ect **SUB**stitution  
**DIR**ect **SUB**stitution = n  
**CON**verge on **TEM**perature = j, ..  
**SIM**ultaneous **CON**vergence **TEM**perature = j, ..  
**CON**vergence **TOL**erance =  
**REPE**at =  
**CAL**culation **SEQ**uence = k, ..  
**RECY**cle **SEQ**uence = k, ..  
**RECY**cle **SEQ**uence 2 = m, ..  
**PR**int **FRE**quency =  
**STO**p after module =  
**RE**verse **CAL**culation  
**RE**verse calculation **MAX**imum iterations = ..  
**RE**verse calculation **TOL**erance = ..

### Recycle Loops Step by Step

#### Recycle Loops STEP 1

##### Enter initial guesses for flowrate, temperature, and pressure

Flowrate guesses FLO (Q units/t units) j =  
 Temperature and pressure guesses TP (T units, P units) j =

#### Recycle Loops STEP 2

##### Enter the maximum number of calculation loops

Maximum number of calculation loops (default is 1, 10 is recommended) MAX =

#### Recycle Loops STEP 3

##### Check an input file (choose any of the options specifications listed below)

Check input file CHE INP  
 Minimum recycle streams specification REC STR =  
 Stream numbers for the minimum number of recycle streams (using Wegstein or Simultaneous Convergence techniques)

##### Convergence method

If a recycle loop is present in the flowsheet and recycle streams have been defined, either by the default unit calculation sequence analysis, CAL SEQ, or REC STR, the Wegstein acceleration technique will be used automatically. Choose one of the options below to specify a different technique.

Simultaneous convergence technique SIM CON  
 Direct substitution DIR SUB  
 Direct substitution for first "n" loops (for SIM CON) DIR SUB = n

##### Convergence on temperature

Stream numbers for convergence on temperature (use only when temperature, rather than component flowrates, changes significantly during convergence) CON TEM = j, ..

Stream temperatures to include as variables in simultaneous convergence technique SIM CON TEM =

**NOTE:** SIM CON, SIM CON TEM, and DIR SUB are disabled if run contains an OPTIMIZE section.

**Convergence tolerance** specification

Convergence tolerance (default is 0.001)

**Case study** calculations

Number of case study trials

**Recycle sequence** specification

Equipment numbers for flowsheet calculation sequence  
OR

Equipment numbers for recycle sequence  
Equipment numbers for recycle loop 2

**Print frequency**

Number of loops between printing

**Stopping calculations**

Last equipment number to be calculated

CON TOL =

REP =

CAL SEQ = k, ..

REC SEQ = k, ..

REC SEQ 2 = m, ..

PRI FRE =

STO =

## Recycle Loops Minimizing Calculations

Since recycle calculations increase the amount of time required to solve a problem and therefore the cost, analyzing your flowsheet to determine if recycle calculations can be eliminated or reduced is beneficial. For example, when all properties of an intermediate stream (component flowrates, temperature and pressure) are known, you should consider entering properties for that stream and use it as a recycle stream.

**Example:**

In the example process flowsheet, stream 1 and stream 4 are known feed streams. Stream 3 flowrates are the same as stream 1, and the temperature of stream 3 is specified; therefore, stream 3 can be entered as a known stream. Stream 3 and stream 4 are the only streams needed to calculate equipment 3. Once equipment 3 is calculated, stream 5 is known and equipment 1 can be calculated and then equipment 2. To solve this problem a TP and FLO command have to be entered in the GENERAL command section for stream 3 along with a RECYCLE STR = 3 command. The GENERAL command section might be coded as follows:

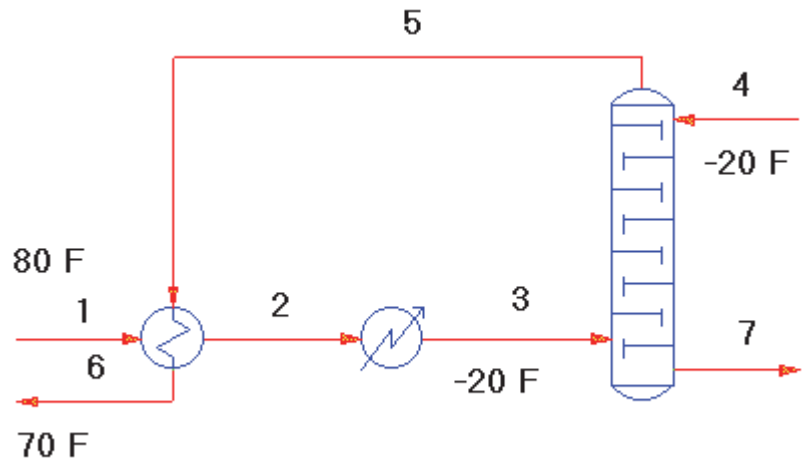
```

GENERAL,
COMPONENTS = 2, 3, 4, 5, 6, 7,
8, 10, 100,
API 100 = 40, AMB 100 = 350,
AMW 110 = 136,
NAM 100 = LEAN OIL,
TP 1 = 80, 800, TP 3 = -20, 800, TP 4 = -20, 820,
FLOW 1 = 9000, 700, 200, 80, 120, 50, 50, 80,
FLOW 3 = FLOW 1,
FLOW 4 = 8*0, 500,
RECYCLE STREAMS = 3,
KVAL, MAX loops = 1,

```

END

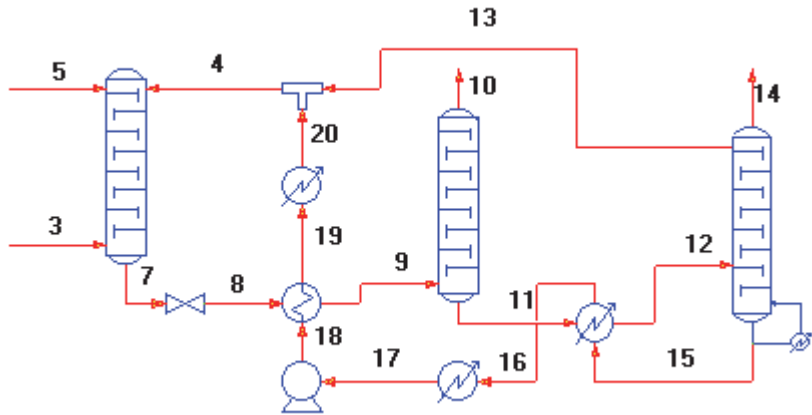
Also, when enough is known about streams used in heat recycling, those streams can be coded as feeds to eliminate the recycle.



# Chapter 10

## Example:

In the process flowsheet for an existing lean oil gas plant, stream 4 represents a material recycle and streams 15 and 18 represent heat recycles. Since streams 15, 16, 17, 18, 19, 20, 4 and 13 represent the lean oil recycle, the component flowrates are known. Equipment 9 is a water cooler and equipment 11 is a refrigerant exchanger, both of which specify the outlet temperature of the lean oil. This means stream 17 and stream 20 can be coded as feed streams and equipment 9 and 11 removed from the simulation.



If you have a good feel for the temperature of stream 15 (the bubble point temperature of the lean oil) you can code it as a feed stream. The following command will eliminate the need for recycle iterations.

```
RECYCLE SEQUENCE = 1,2,3,4,5,6,7,8,
```

The order of equipment calculations (and recycle streams) chosen by DESIGN II can be found in your output under the heading UNIT CALCULATION SEQUENCE ANALYSIS. An input example with its corresponding UNIT CALCULATION report is shown on the following pages.

### \*MEA SAMPLE PROBLEM

C-

C- CONTACTOR

C-

```
DIStill 1 = CONT,1,2,-3,-4, ABSorber, TRAYS = 7,LOCation FEEd = 1,8,
PREss TOP = 914.7,
TEMP TOP gue = 110, TEMP BOT gue = 140, PROducts = 0,10130,
SAVE PROfiles, SAVe MATrix,
```

C-

C- HEAT EXCHANGERS

C-

```
HEAT EXCh 2 = BOTTOM EXCH,4,13,-5,-14, TEMP OUT = 220,
HEAT EXCh 3 = COOL,14,-1, TEMP OUT = 100,
```

C-

C- REGENERATOR

C-

```
DIStill 5 = REGEN,6,-7,-8,
PARTial cond,
TRAYS = 6,
LOCation FEEd = 2,
PREss TOP = 22,
TEMP TOP gue = 230,
TEMP BOT gue = 260,
PROducts = 0,9500,
COMp CONv = 10,2,
REFlux = 2.5,
RECOvery TOP 62 = 20.,
DVS=.4,
SAVE PROfiles,
```

C-

C- DROP PRESSURE FOR REGENERATOR

C-

```
VALve 4 = LETDN,5,-6, PREssure OUT = 22,
```

C-

C- RAISE PRESSURE FOR CONTACTOR

C-

```
PUMp 6 = RECOMP,12,-13, PREssure OUT = 914.7
```

C-

C- WATER MAKEUP

C-

```
COMSPL20 = MAKE,8,-9,-10, REC TOP = 3*1,0,1,
MIX 7 = WATR,9,11,-12,
```

C-

C- GENERAL SECTION

C-

```
GENeral,
COMp = 2,49,50,62,4155,
FLOW 1 = 0,62.4,1.21,9440.67,489.6, TP 1 = 100,914.7,
```

```

FLOW 2 = 5351.87,125.76,31.32,0,0, TP 2 = 90,914.7,
FLOW 11 = 3*0,9440.67,0, TP 11 = 236.26,22,
MDEAK, MDEAH,
CHEck INPut

```

END

```

++++UNIT CALCULATION SEQUENCE ANALYSIS *****BEGIN RECYCLE LOOP 1
*****RECYCLE STREAM: 8
CALCULATE MAKE : COMSPL 20
CALCULATE WATR : MIX 7
CALCULATE RECO : PUM 6
*****RECYCLE STREAM: 1
CALCULATE CONT : DIS 1
CALCULATE BOTT : HEAEXC 2
CALCULATE COOL : HEAEXC 3
CALCULATE LETD : VAL 4
CALCULATE REGE : DIS 5
*****END RECYCLE LOOP 1

```

Before running this case you would add FLO and TP commands for streams 8 and 1 (the recycle streams), a MAX= command, a CON TOL= command, and you would remove the CHEck INPut command.

## Recycle Loops Review of DESIGN II Output

DESIGN II Output Includes A Material Balance Summary Which Is Printed after the equipment summary. You can refer to this page for a quick review of individual component material balance as well as the overall material balance. The summary shown on the following page is from a converged recycle loop calculation using a CONvergence TOLerance of 0.01.

### M A T E R I A L   B A L A N C E   S U M M A R Y

COMPONENT NAME	FEED (S) KGMOL	PRODUCT (S) KGMOL	DIFFERENCE KGMOL	REL. ERROR
METHANE	113.4	113.4	0.0000E+00	0.0000E+00
ETHANE	23.59	23.59	0.0000E+00	0.0000E+00
PROPANE	54.88	54.88	0.0000E+00	0.0000E+00
I-BUTANE	7.257	7.257	0.0000E+00	0.0000E+00
N-BUTANE	0.4536	0.4536	0.0000E+00	0.0000E+00
TOTAL	199.6	199.6	0.0000E+00	0.0000E+00
FLOWRATE /HR				

**NOTE:** Be sure to check the material balance summary for a converged recycle loop because the convergence tolerance error is checked on recycle stream(s) from iteration to iteration, not on overall material balance. If there is a problem, you may want to choose another stream for recycle acceleration or tighten convergence tolerance (CON TOL=). For flowsheets involving numerous equipment calculations (especially if rigorous distillation columns or setpoint controllers are involved), you can quickly review your output by printing the INDEX. This will tell you whether DISTillation columns converged in each iteration of the loop, whether setpoint CONTrollers converged, and whether the recycle loop converged. The page number where specific information is reported is included in the index, so you can start printing your output file at the last iteration. This is particularly useful if you are printing your output on a low-speed terminal. A sample index is shown below and on the following pages.

PAGE	INDEX OF FLOWSHEET CALCULATIONS			
6	++++ BEGIN ITERATION	1 OF RECYCLE LOOP	1	++++
6	DIS 1	(CONT) CONVERGED NORM=		0.5779E-06
11	PROFILES			
14	PRODUCTS			
21	HEAEXC 2	(BOTT)		
21	VAL 4	(LETD)		
21	DIS 5	(REGE) CONVERGED NORM=		0.9455E-07
26	PROFILES			
27	PRODUCTS			
29	COMSPL 20	(MAKE)		
29	MIX 7	(WATR)		
29	PUM 6	(RECO)		
29	HEAEXC 3	(COOL)		
30	++++ BEGIN ITERATION	2 OF RECYCLE LOOP	1	++++
30	DIS 1	(CONT) CONVERGED NORM=		0.3003E-06
35	PROFILES			
38	PRODUCTS			
45	HEAEXC 2	(BOTT)		
45	VAL 4	(LETD)		
45	DIS 5	(REGE) CONVERGED NORM=		0.2032E-07
50	PROFILES			

## Chapter 10

```
51          PRODUCTS
52  COMSPL      20      (MAKE)
53  MIX         7      (WATR)
53  PUM         6      (RECO)
53  HEAEXC     3      (COOL)
54  ++++ BEGIN ITERATION 3 OF RECYCLE LOOP 1 ++++
54  DIS         1      (CONT) CONVERGED NORM= 0.1071E-06
59          PROFILES
62          PRODUCTS
69  HEAEXC     2      (BOTT)
69  VAL         4      (LETD)
69  DIS         5      (REGE) CONVERGED NORM= 0.2303E-07
74          PROFILES
75          PRODUCTS
77  COMSPL     20      (MAKE)
77  MIX         7      (WATR)
77  PUM         6      (RECO)
77  HEAEXC     3      (COOL)
78  +++ BEGIN ITERATION 4 OF RECYCLE LOOP 1 ++++
78  DIS         1      (CONT) CONVERGED NORM= 0.5491E-06
83          PROFILES
86          PRODUCTS
93  HEAEXC     2      (BOTT)
93  VAL         4      (LETD)
93  DIS         5      (REGE) CONVERGED NORM= 0.2018E-06
98          PROFILES
99          PRODUCTS
101 COMSPL     20      (MAKE)
101 MIX         7      (WATR)
101 PUM         6      (RECO)
101 HEAEXC     3      (COOL)
103 +++BEGIN ITERATION 5 OF RECYCLE LOOP 1 ++++
103 DIS         1      (CONT)
108          PROFILES
111          PRODUCTS
118 HEAEXC     2      (BOTT)
118 VAL         4      (LETD)
118 DIS         5      (REGE) CONVERGED NORM= 0.1419E-07
123          PROFILES
124          PRODUCTS
126 COMSPL     20      (MAKE)
126 MIX         7      (WATR)
126 PUM         6      (RECO)
126 HEAEXC     3      (COOL)
128 +++BEGIN ITERATION 6 OF RECYCLE LOOP 1 ++++
128 DIS         1      (CONT) CONVERGED NORM= 0.2172E-06
133          PROFILES
136          PRODUCTS
143 HEAEXC     2      (BOTT)
143 VAL         4      (LETD)
143 DIS         5      (REGE) CONVERGED NORM= 0.8411E-07
148          PROFILES
151          PRODUCTS
158 COMSPL     20      (MAKE)
158 MIX         7      (WATR)
158 PUM         6      (RECO)
158 HEAEXC     3      (COOL)
160 ++LOOP 1 HAS CONVERGED AFTER 6 ITERATIONS +++
161 STREAM SUMMARY
166 EQUIPMENT SUMMARY - HEAT EXCHANGERS
167 EQUIPMENT SUMMARY - PUMPS
171 MATERIAL BALANCE SUMMARY
172 DETAILED STREAM PRINT
```

### Recycle Loops Example Using Case Study Repeat Command

Consider using the flowsheet Case Study option also. The values stored in SPECS will be used for mass purity specifications for ethane in the bottom product. The values stored in PROPs will be as specifications for the Value outlet pressure (VALve1) and for the column top tray pressure (after subtracting 5 psia). Flowsheet calculations will be REPEATED 5 times. DISTillation product results will be copied to flowsheet streams 101-105 (overhead) and 201-205 (bottoms).

AB123.

\* ETHANE RECOVERY CASE STUDY

C-

C- DISTILLATION COLUMN T1 - CHECK DIFFERENT ETHANE PURITY SPECS AND COLUMN PRESSURES

C-



```

VALve 1 = LETDOWN,1,-2, PREssure OUT =
F-   PRE
F-   DIMENSION SPECS(5)
F-   DIMENSION PROPS(5)
F-   COMMON /MYVARS/ ISP,ISTR,SPEC
F-   DATA SPECS /.001, .003, .003, .005, .007/
F-   DATA PROPS /345.0, 345.0, 334.7, 334.7, 300.0/
F-   ISTR = ISTR + 1
F-   ISP = ISP + 1
F-   SPEC = SPECS(ISP)
F-   SET (VAL(1),PRE OUT) = PROPS(ISP)
F-   SET (DIS(2),PRE TOP) = PROPS(ISP) - 5.0
DIStillation 2 = T1,2,-3,-4, PARTial
LOCation FEEd = 10, PREssure TOP = 340
DELta = 8, TEMperature TOP = 30, TEMperature BOTtom = 200
TRAys = 20 ,PURity BOTtom (MASS) 3 = .001
PROducts = 0,260, SAVE TEMperature profile, SAVE VAPor profile
REFlux = 1.5, PRint SWitch = 0 F-   DURING
F-   COMMON /MYVARS/ ISP,ISTR,SPEC
F-   SUM=0.0
F-   DO 25 I=1,9
F-   SUM=FLOWL(I,1)*GET(BANK(AMW),POS(I)) + SUM
F-   25 CONTINUE
F-   C2FLOW=FLOWL(3,1)*GET(BANK(AMW),POS(3))
F-   C2PUR=C2FLOW/SUM
F-   EPS(1)=(C2PUR -SPEC)/SPEC
C-   VAPOR PRODUCT STREAM RESULTS ARE STORED IN STREAMS 101 - 105
C-   LIQUID PRODUCT STREAM RESULTS ARE STORED IN STREAMS 201 -
C-   205
MIXer 3 = OVHD
PRE
F-   DIMENSION PROP (10)
F-   DATA PROF/101, 102, 103, 104, 105, 202, 203, 204, 205
F-   COMMON /MYVARS/ ISP,ISTR,SPEC
F-   JSTR = 100 + ISTR
F-   KSTR = 200 + ISTR
F-   CALL COPSTR(3,JSTR)
F-   CALL COPSTR(4,KSTR)
GENeral,
COMponents = 49,2,3,4,5,6,7,8,10
FLOW 1 = .2, 3.2, 156.7, 113.8, 38.9, 46.4, 20, 16, 30
TP (PSIG) 1 = 121.77, 350
C-   THERMODYNAMIC DATA
SOAVEK, SOAVEH, STDD
C-   CASE STUDY INFORMATION
CALculation SEQuence = 1,2,3, REPEAT = 5
C-   PRINT RESTRICTIONS
PRint STReams = 1,101,102,103,104,105,201,202,203,204,205
END

```



# Chapter 11: Input Units

A convenient and powerful feature of DESIGN II is the total control of input and output units. Input specifications can be entered in a wide variety of units. These input units are controllable at the keyword command level or may be altered to affect the input as a whole. Refer to Chapter 6.4 for more information on output units.

Four choices are available for specifying input units to DESIGN II.

- Enter specific unit options for individual keyword commands.
- Enter unit options for specific input quantities, e.g., all input temperatures.
- Enter unit option for the entire input e.g., US, Metric, SI, Europe units.

## Input Units: Keyword Unit Specification

All of the keyword input commands for DESIGN II indicate which category of units options is to be used for each specification. Input specifications for DESIGN II can be entered in just about any units you wish to use.

The codes for available units options are presented by category in *Input Units: Options*. Simply choose the units you want to use and enter the units code. Remember several important points about specifying input units at the keyword command level:

- Specifying units for input specifications is not necessary if you want to use standard default units. When no units are specified, the program automatically uses the units shown under the column headed DEFAULT in *Input Units (Default) for Global Systems*.
- Input unit specification at the keyword command level takes priority over input unit specification at any other level.
- Specifying input units at the keyword command level does not affect the output units in any way.

## Input Units: Individual Quantity Unit Specification

A second method for specifying input units is to assign selected units for individual quantities. For example, all temperature inputs can be specified in one set of units while all other quantities remain in the default set. This technique of specifying input units has the following key features:

- Unit options selected in this fashion set not only the input units but the output units for the individual quantity as well.
- This technique overrides any units specification made with a global command, i.e., METric UNIts or SI UNIts or EUROPE UNIts, but is overridden itself by a units specification made at the keyword command level.
- Not all input quantities can be specified in this way.
- The commands entered in the GENeral section of the input file to specify units for individual quantities are:

**QU**antity **UN**Its =

Enter Units Code to specify molar flowrate units for input and output. (See *Input Units: Options* for Units Code)

**TEM**perature **UN**Its =

Enter Units Code to specify temperature units for both input and output. (See *Input Units: Options* for Units Code)

**PRE**ssure **UN**Its =

Enter Units Code to specify pressure units for both input and output. (See *Input Units: Options* for Units Code)

**ENT**halpy **UN**Its =

Enter Units Code to specify enthalpy units for both input and output. (See *Input Units: Options* for Units Code)

**TIM**e **UN**Its =

Enter Units Code to specify time units for both input and output. (See *Input Units: Options* for Units Code)

**LEN**gth **UN**Its =

Enter Units Code to specify length units for both input and output. (See *Input Units: Options* for Units Code)

## Input Units: Command Summary

### Individual Quantity Unit Specification

(Set units on selected quantities for input and output)

**QU**antity **UN**Its =

**TEM**perature **UN**Its =

**PRE**ssure **UN**Its =

**ENT**halpy **UN**Its =

**TIM**e **UN**Its =

**LEN**gth **UN**Its =

### Global Unit Specification

(Set units for ALL input and output)

**MET**ric **UN**Its

**SI** **UN**Its

**EUROPE** **UN**Its

**VOL**ume **ST**andard conditions = **STP** or **NTP**

## Input Units: Step by Step

Command Level Priority Table

# Chapter 11

## Input/Output

Keyword Input (e.g., TP (C,ATM) j =)  
 Individual Input/Output (e.g., TIM UNI =)  
 Global Input/Output (e.g., SI UNI)  
 Global Input/Output (e.g., MET UNI)  
 Global Input/Output (e.g., EUR UNI)

## Output

Individual Output (e.g., TIM UNI OUT =)  
 Individual Input/Output (e.g., PRE UNI =)  
 Global Output (e.g., SI UNI OUT)  
 Global Output (e.g., MET UNI)  
 Global Output (e.g., EUR UNI)

The above table shows the override order of the unit specifications, i.e. commands appearing higher in each column will override the units specified using any command lower in the column.

**Input units may be entered with any command keyword. The required units for the command will be listed with the keyword.**

To input temperature and pressure units for stream 1 different than the default degrees F and PSIA, e.g. 1000 degrees Rankine and 150 millimeters of mercury, enter the following command in the GENeral section:

**TP (R,MMHG) 1 = 1000, 150**

See Table 1 for default unit codes and Table 2 for all unit codes

## Input Units STEP 1

**Select any of the optional commands listed below to specify both INPUT AND OUTPUT units for individual quantities. Place selection(s) in the GENeral section of the input file.** Individual quantity unit specification (select any of the following options).

Molar flowrate units for input and output  
 Temperature units for both input and output  
 Pressure units for both input and output  
 Enthalpy units for both input and output  
 Time units for both input and output  
 Length units for both input and output

**QUA UNI =**  
**TEM UNI =**  
**PRE UNI =**  
**ENT UNI =**  
**TIM UNI =**  
**LEN UNI =**

## Input Units STEP 2

**Select either command at the right to specify units for ALL input and output units. Place command in the GENeral section of the input file. Select one of the following options:**

See **Input Units: Options** for units code

Metric units for ALL input and output quantities  
 SI units for ALL input and output quantities  
 Europe units for ALL input and output quantities  
 Use Volume Standard conditions as STP (or) NTP for ALL input or output quantities using Metric or SI unit system.

**MET UNI**  
**SI UNI**  
**EURope UNI**  
**VOL STA = STP or NTP**

## Input Units: Global Unit Specification

The final method for specifying input units is to select an overall units system to be used for **ALL** input and output. The GENeral section commands for selecting this method are:

### METric UNIts

Enter this command to specify metric units for ALL input and output quantities.

### SI UNIts

Enter this command to specify SI units for ALL input and output quantities.

### EURope UNIts

Enter this command to specify SI units for ALL input and output quantities. Volume standard condition is NTP (default).

### VOLume STAndard condition = STP or NTP

Enter this command to specify one of the volume standard conditions: STP (60 F, 14.696 psia) or NTP (0 C, 1 atm). This applies only for Metric and SI unit systems. US unit system is always calculated at STP conditions.

## Input Units: (Default) for Global Systems

Quantity	Default	Metric	SI
Q units (quantity)	LBMOL	KGMOL	KGMOL
P units (pressure)	PSIA	KG/CM2	KPA/MPA
T units (temperature)	F	C	K
H units (enthalpy)	BTU	KCAL	KJ
L units (length)	FT	M	M
p units (power)	HP	METric HP	WAtts
t units (time)	HR	HR	SEC
U units (heat transfer)	BTU/HR/FT2/F	KCAL/HR/M2/C	KJ/SEC/M2/K

G units (gravity)	API*	SPG	SPG
R units (rotating speed)	RPM	RPM	RPS
k units (thermal conductivity)	BTU/HR/FT/F	KCAL/HR/C	KJ/S/M/K
V units (kinematic viscosity)	CST		
V units (dynamic viscosity)	CP	CP	NS/M2

\*Input only, stream summaries and detailed stream summaries will report specific gravity or densities.

## Input Units: Options

**NOTE:** For engineering convenience, Design II uses KPA and KJ as SI units rather than the strict SI standard units, pascals and joules.

Quantity (Q units)			Rotating Speed (R units)		
<b><u>Molar Q Units</u></b>			RPM	Default	Revolutions per minute
LBMOL	Default	Pound moles	RPS	SI Units	Revolutions per second
GMOL		Gram moles	<b><u>Pressure (P units)</u></b>		
KGMOL	Metric,SI	Kilogram moles	PSIA	Default	Pounds per square inch, absolute
<b><u>Mass Q Units</u></b>			PSIG		Pounds per square inch, gauge
LB		Pounds	ATM		Atmosphere
G		Grams	MMHG		Millimeters of mercury
KG		Kilograms	BAR		Bars
TON		Short tons	MMH2O		Millimeters of water
TONNE		Metric tons	INH2O		Inches of water
<b><u>Liquid Volume Q Units</u></b>			KG/CM2	Metric	Kilograms per square centimeter
GAL		Gallons (liquid) STP	KG/M2		Kilograms per square meter
BBL		Barrels (liquid) STP	DY/CM2		Dynes per square centimeter
LIT		Liters (liquid) NTP	G/CM2		Grams per square centimeter
M3LIQ		Cubic meters (liquid) NTP	PA		Pascals
M3LIQSTP		Cubic meters (liquid) STP	KPA	SI Units	Kilopascals
FT3LIQSTP		Cubic feet (liquid) STP	MPA	SI Units	Megapascals
<b><u>Vapor Volume Q Units</u></b>			ATMG		Atmosphere (gauge)
SCF		Standard cubic feet (vapor)	BARG		Bars (gauge)
MSCF		Thousand standard cubic feet (vapor)	MMH2OG		Millimeters of water (gauge)
MMSCF		Million standard cubic feet (vapor)	INH2OG		Inches of water (gauge)
M3API		Cubic meters (vapor at 15C and 1 atm)	KG/CM2G		Kilograms per square centimeter (gauge)
M3VAPAPI		Cubic meters (vapor at API 15C and 1 atm)	DY/CM2G		Dynes per square centimeter (gauge)
M3VAP		Cubic meters (NTP vapor)	G/CM2G		Grams per square centimeter (gauge)
M3VAPSTP		Cubic meters (STP vapor)	PAG		Pascals (gauge)
<b><u>Power (p units)</u></b>			KPAG		Kilopascals (gauge)
HP	Default	Horsepower	MPAG		Megapascals
KW	Metric &	Kilowatts	KG/M2G		Kilograms per square meter (gauge)
WA	SI Units	Watts	<b><u>Length, Area, Volume (L Units)</u></b>		
<b><u>Time (t units)</u></b>			FT	Default	Feet
HR	Default, Metric	Hours	CM		Centimeters
SEC	SI Units	Seconds	M	Metric, SI Units	Meters
MIN		Minutes	MM		Millimeters
DAY		Days	YD		Yards
YR		Years	IN		Inches
<b><u>Enthalpy Units</u></b>			MILE		Miles (LINE and SIZE LINES only)
BTU	Default	British thermal units	<b><u>Viscosity Units (V units)</u></b>		
CAL		Calories	<b><u>Dynamic Viscosity Options</u></b>		
KCAL	Metric	Kilocalories	CP	Default, Metric	Centipoise
FTLB		Foot-Pounds	POISE		Poise
J		Joules	LB/FT.S		Pounds per foot per second
KJ	SI	Kilojoules	KG/M.S		Kilogram per meter per second
MJ		Megajoules	NS/M2		Newton Seconds per meter squared
			PA.S		Pascal Seconds

# Chapter 11

## Heat Transfer (U units)

BTU/HR/FT2/F Default  
 KCAL/HR/M2/C Metric Units  
 KJ/SEC/M2/K SI Units

## Gravity (G units)

API Default API gravity  
 SPG Metric, SI Units Specific gravity

## Kinematic Viscosity Options

CST Centistokes  
 FT2/S Foot squared per second  
 SUS Saybolt Universal Seconds  
 SFS Saybolt Furol Seconds  
 RED1 Redwood No. 1 Seconds  
 RED2 Redwood Admiralty  
 M2/S Meter squared per Second

## Thermal Conductivity (k units)

BTU/HR/FT/F Default  
 KCAL/HR/M/C Metric Units  
 KJ/S/M/K SI Units

**NOTE:** Standard conditions are:  
 STP 60F 14.696 PSIA  
 NTP 0 C 1 ATM  
 API 15 C 1 ATM

## Input Units: Examples

### Input Units: Discharge Pressure Units

Enter a discharge pressure of 70 kilograms per square centimeter for a compressor. Assume that the rest of the input is being created with default input units. The compressor outlet pressure command is listed as:

**PRE**ssure **OUT** (P units) =

The units code for kilograms per square centimeter (from the P units category) is KG/CM2, so the command is entered as follows:

**PRE OUT** (KG/CM2) = 70

This compressor outlet pressure specification pertains to the data input only. The outlet stream data in the printout is not affected by this command. It will still be reported in default units.

### Input Units: Temperature and Pressure Units

Enter the temperature (80.5 C) and pressure (1002 millimeters of mercury) for a feed defined as flowsheet stream 1. Assume that the rest of the input is being created with default input units. The command for the temperature and pressure of a feed is listed as:

**TP** (T units, P units) j =

The units code for Centigrade is C and for millimeters of mercury is MMHG. Therefore, the command is entered as follows:

**TP** (C, MMHG) 1 = 80.5, 1002

Again, the units specification at the keyword command level does nothing to affect the units used in the output.

### Input Units: Default Temperature and Pressure Units

If the temperature and pressure of the stream in Example 2 are to be specified in the default units F and PSIA, no input unit specification would be required. The command would be:

**TP** 1 = 176.9, 19.4

# Chapter 12: Output Units

A convenient and powerful feature of DESIGN II is the total control of input and output units. Output unit control can be entirely independent of the input units. Again, a wide range of units is available. Additionally, DESIGN II allows the definition of standard conditions (temperature and pressure) for property product volumes. Unless otherwise directed by a specific command, DESIGN II defaults to American units for both input and output. Refer to Chapter 6.3 for more information on input units

The units contained in the program printout can be completely independent of the input units specified. If the default output units are not satisfactory, change them by entering commands in the GENERAL section. If no commands are entered, all data will be reported in default units as described in *Output Units By System*. Two methods can be used to specify output units.

1. Enter unit options for specific output quantities , e.g. all output temperatures.
2. Enter a global unit option for the entire output , e.g. Metric, SI, Europe units.

## Output Units: Individual Output Quantity Unit Specification

The first method for specifying output units is to assign individual quantities selected units. For example, all temperature outputs can be specified in one set of units while all other quantities remain in the default set. This technique overrides any output units specification made with a global output units command, i.e., SI UNI OUT, MET UNI OUT and EUROPE UNI OUT commands. See *Output Units: Options* for Units Code.

The commands entered in the GENERAL section to specify output units for individual quantities are:

### QUANTITY UNITS OUT =

Enter Units Code to specify component mass, volume or molar flowrate units for the stream summary. If molar units are specified, they will also be used for detailed stream printout. (See *Output Units: Options* for Units Code)

### TEMPERATURE UNITS OUT =

Enter Units Code to specify temperature units for output. (See *Output Units: Options* for Units Code)

### PRESSURE UNITS OUT =

Enter Units Code to specify pressure units for output. (See *Output Units: Options* for Units Code)

### ENTHALPY UNITS OUT =

Enter Units Code to specify enthalpy units for output. (See *Output Units: Options* for Units Code)

### TIME UNITS OUT =

Enter Units Code to specify time units for output. (See *Output Units: Options* for Units Code)

### LENGTH UNITS OUT =

Enter Units Code to specify length, area or volume units for output. (See *Output Units: Options* for Units Code)

### DENSITY UNITS OUT =

Enter Units Code to specify density units for output. (See *Output Units: Options* for Units Code)

### VAPOR UNITS OUT =

Enter Units Code to specify vapor flow units for detailed stream printout. Select molar, mass, or volume Q units. This command cannot be used alone. It must be used with the LIQ UNI OUT command. (See *Output Units: Options* for Units Code)

### LIQUID UNITS OUT =

Enter Units Code to specify liquid flow units for detailed stream printout. Select molar, mass, or volume Q units. This command cannot be used alone. It must be used with the VAP UNI OUT command. (See *Output Units: Options* for Units Code)

### VAPOR VOLUMETRIC UNITS OUT =

Enter Units Code to specify vapor flow units for detailed stream printout. Select molar, mass, or volume Q units. (See [Output Unit Options](#) for Units Code)

### VAPOR VOLUMETRIC TIME UNITS OUT =

Enter units code for the vapor flow time units for detailed stream printout. (See [Output Unit Options](#) for Units Code)

### STP VAPOR VOLUMETRIC UNITS OUT =

Enter Units Code to specify standard vapor flow units for detailed stream printout. Select molar, mass, or volume Q units. (See [Output Unit Options](#) for Units Code)

### STP VAPOR VOLUMETRIC TIME UNITS OUT =

Enter units code for the standard vapor flow time units for detailed stream printout. (See [Output Unit Options](#) for Units Code)

### LIQUID UNITS OUT =

Enter Units Code to specify liquid flow units for detailed stream printout. Select molar, mass, or volume Q units. (See [Output Unit Options](#) for Units Code)

### LIQUID TIME UNITS OUT =

Enter units code for the liquid flow time units for detailed stream printout. (See [Output Unit Options](#) for Units Code)

### STP LIQUID UNITS OUT =

Enter Units Code to specify standard liquid flow units for detailed stream printout. Select molar, mass, or volume Q units. (See [Output Unit Options](#) for Units Code)

## Chapter 12

### **STP LIQuid TIME UNIts OUT =**

Enter units code for the standard liquid flow time units for detailed stream printout. (See [Output Unit Options](#) for Units Code)

### **VIScosity UNIts OUT =**

Enter Units Code to specify viscosity units for detailed stream printout. (See *Output Units: Options* for Units Code)

### **PETroleum UNIts OUT =**

Enter this command when you wish flowrates normally reported in gallons per minute to be reported in barrels per day. For use with default output units only. (See *Output Units: Options* for Units Code)

### **DUTy UNIts OUT =**

Enter Units Code to specify duty units on all exchanger printouts. (See [Output Unit Options](#) for Units Code). NOTE: the DUT UNI OUT command changes ALL enthalpy/time values. When this command is not used the program will use enthalpy/time units out.

### **POWer UNIts OUT =**

Enter Units Code to specify power units on all compressor & expander printouts. (See [Output Unit Options](#) for Units Code)

## Output Units: Global Output Unit Specification

The second method for specifying output units is to select an overall units system to be used for **ALL** output. These commands change all output units to the specified system. The units for each system are shown in *Output Units By Systems*. The GENERAL section commands for selecting this method are:

### **AMErican UNIts OUT**

Specifies American or US units system for all output

### **SI UNIts OUT**

Specifies SI units system for all output.

### **METric UNIts OUT**

Specifies metric units system for all output.

### **EUROpe UNIts OUT**

Specifies Europe units system for all output.

### **Example 1.**

If you want all output data reported in the standard metric units, enter the command:

```
MET UNI OUT
```

## Output Units: Command Summary

### Individual Output Unit Specification

(Set units on selected quantities for output only)

**QUANtity UNIts OUT =**

**TEMperature UNIts OUT =**

**PREssure UNIts OUT =**

**ENThalpy UNIts OUT =**

**TIMe UNIts OUT =**

**LENGth UNIts OUT =**

**DENSity UNIts OUT =**

**VAPor UNIts OUT =**

**VAPor TIMe UNIts OUT =**

**STP VAPor UNIts OUT =**

**STP VAPor TIMe UNIts OUT =**

**LIQuid UNIts OUT =**

**LIQuid TIMe UNIts OUT =**

**STP LIQuid UNIts OUT =**

**STP LIQuid TIMe UNIts OUT =**

**PETroleum UNIts OUT**

**DUTy UNIts OUT =**

**POWer UNIts OUT =**

### Global Output Unit Specification

(Set units for ALL output quantities)

**AMErican UNIts OUT**

**SI UNIts OUT**

**METric UNIts OUT**

**EUROpe UNIts OUT**

## Output Units: Step by Step

### **Command Level Priority Table**

#### **Input/Output**

Keyword Input (e.g., TP (C,ATM) j =)

#### **Output**

Individual Output (e.g., TIM UNI OUT =)



Individual Input/Output (e.g., TIM UNI =)  
 Global Input/Output (e.g., SI UNI)  
 Global Input/Output (e.g., MET UNI)  
 Global Input/Output (e.g., EUROPE UNI)

Individual Input/Output (e.g., PRE UNI =)  
 Global Output (e.g., SI UNI OUT)  
 Global Output (e.g., MET UNI OUT)  
 Global Output (e.g., EUR UNI OUT)

The above table shows the override order of the unit specifications, i.e. commands appearing higher in each column will override the units specified using any command lower in the column.

## Output Units STEP 1

**Select any of the optional commands listed below to specify OUTPUT units for individual quantities. Place selection(s) in the GENERAL section of the input file**

See Table 3 for units code

Component mass, volume or molar flowrate units for the stream summary  
 Temperature units for output  
 Pressure units for output  
 Enthalpy units for output  
 Time units for output  
 Length, area or volume units for output  
 Density units for output  
 Vapor flow units for detailed system printout  
 Vapor flow time units for detailed stream printout  
 Standard vapor flow units for detailed stream printout  
 Standard vapor flow time units for detailed stream printout

Liquid flow units for detailed stream printout  
 Liquid flow time units for detailed stream printout  
 Standard liquid flow units for detailed stream printout  
 Standard liquid flow time units for detailed stream printout

Flowrates reported in barrels per day (for use with default units **only**)  
 Duty units on all exchanger printouts. NOTE: the DUT UNI OUT command changes ALL enthalpy/time values. When this command is not used the program will use enthalpy/time units out.

Units Code to specify power units on all compressor & expander printouts.

QUA UNI OUT =  
 TEM UNI OUT =  
 PRE UNI OUT =  
 ENT UNI OUT =  
 TIM UNI OUT =  
 LEN UNI OUT =  
 DEN UNI OUT =  
 VAP UNI OUT =  
 VAPor TIME UNIts OUT =  
 STP VAPor UNIts OUT =  
 STP VAPor TIME UNIts OUT =  
 LIQUid UNIts OUT =  
 LIQUid TIME UNIts OUT =  
 STP LIQUid UNIts OUT =  
 STP LIQUid TIME UNIts OUT =  
 PET UNI OUT =  
 DUT UNI OUT =

POW UNI OUT =

## Output Units STEP 2

**Select any of the optional commands at the right to specify ALL output units. Place command in the GENERAL section of the input file (select any of the following options).**

See *Output Units By System*

American units system for all output  
 SI units system for all output  
 Metric units system for all output  
 Europe units system for all output

AME UNI OUT  
 SI UNI OUT  
 MET UNI OUT  
 EUR UNI OUT

## Output Units: Examples

### Output Units: Global

If you want all output data reported in metric units except for temperature, which you want in degrees Kelvin, enter:

```
MET UNI OUT
TEM UNI OUT = K
```

### Output Units: Quantity

If you want all output in default units except for Stream Summary component flowrates which you want in kilogram-moles per hour, you would enter:

```
QUA UNI OUT = KGMOL
```

### Output Units: Global SI Units with Time Units

If you are using the SI units, but want flowrates reported in kilogram-moles per hour instead of kilogram-moles per second, you would enter:

```
SI UNI OUT
```

# Chapter 12

TIM UNI OUT = HR

## Output Units: Liquid and Vapor Outlet Units

If you want liquid flow reported in kilograms and vapor flow reported in API cubic meters, you would enter:

LIQ UNI OUT = KG,  
VAP UNI OUT = M3API

**NOTE:** These commands cannot be entered single; both must appear in the input file.

## Output Units: Options

<b>Molar Quantity Units</b>			<b>Enthalpy Units</b>		
LBMOL	Default	Pound-moles	BTU	Default	British thermal units
GMOL		Gram-moles	CAL		Calories
KGMOL	SI, Metric	Kilogram-moles	KCAL	Metric	Kilocalories
<b>Mass Quantity Units</b>			FTLB		Foot-Pounds
LB		Pounds	J		Joules
G		Grams	KJ	SI	Kilojoules
KG		Kilograms	MJ		Megajoules
TON		Short tons	<b>Duty Units</b>		
TONNE		Metric tons	BTU/HR	Default	British thermal units per hour
<b>Volume Quantity Units</b>			KCAL/HR		Kilocalories per hour
<i>Vapor:</i>			KW		Kilowatts
SCF		Standard cubic feet	CAL/MIN		Calories per minute
MSCF		Thousand standard cubic feet	WA		Watts
MMSCF		Million standard cubic feet	MJ/HR		Megajoules per hour
ACF		Actual cubic feet	KJ/HR		Kilojoules per hour
MACF		Thousand actual cubic feet	KJ/SEC		Kilojoules per second
MMACF		Million actual cubic feet	J/SEC		Joules per second
<b>Note:</b>			<b>Power Units</b>		
The SCF and ACF units are completely equivalent.			HP		Horsepower
You get ACF at T-P and SCF at STP.			KW		Kilowatts
M3 VAP NTP		Cubic meters NTP	WA		Watts
M3 VAP STP		Cubic meters STP	HP METRIC		Horsepower Metric
M3 VAP API		Cubic meters API	<b>Time Units</b>		
<b>Note:</b>			HR	Default, Metric	Hours
Defaults to M3 VAP NTP if only M3 or M3 VAP is entered.			SEC	SI	Seconds
<i>Liquid:</i>			MIN		Minutes
BBL STP		Liquid barrels	DAY		Days
GAL STP		Liquid gallons	YR		Years
FT3 LIQ STP		Cubic feet STP	<b>Length, Area, Volume Units</b>		
M3 LIQ STP		Cubic meters STP	FT	Default	Feet
M3 LIQ NTP		Cubic meters NTP	CM		Centimeters
<b>Note:</b> Defaults to M3 LIQ NTP if only M3 or M3 LIQ is entered.			M	SI, Metric	Meters
LIT NTP		Liters NTP	MM		Millimeters
<b>Temperature Units</b>			YD		Yards
F	Default	Fahrenheit	IN		Inches
C	Metric	Celsius	<b>Density Units</b>		
R		Rankine	LB/FT3	Default	Pounds per cubic foot
K	SI	Kelvin	G/CM3		Grams per cubic centimeter
<b>Pressure Units</b>			KG/M3	SI, Metric	Kilograms per cubic meter
PSIA	Default	Pounds per square inch, absolute	LB/GAL		Pounds per gallon
PSIG		Pounds per square inch, gauge	<b>Viscosity Output Units</b>		
ATM		Atmospheres	<b>Dynamic Viscosity Options</b>		
MMHG		Millimeters of mercury	CP	Default, Metric	Centipoise
MMH2O		Millimeters of water	POISE		Poise
INH2O		Inches of water	LB/FT.S		Pound per foot per second
			KG/M.S		Kilogram per meter per second
			NS/M2		Newton Seconds per meter squared
			PA.S		Pascal Seconds

BAR		Bars	<b>Kinematic Viscosity Options</b> CST Centistokes FT2/S Foot squared per second SUS Saybolt Universal Seconds SFS Saybolt FuroI Seconds RED1 Redwood No. 1 Seconds RED2 Redwood Admiralty M2/S Meter squared per Second
KG/CM2	Metric	Kilograms per square centimeter	
KG/M2		Kilograms per square meter	
DY/CM2		Dynes per square centimeter	
G/CM2		Grams per square centimeter	
PA		Pascals	
KPA	SI	Kilopascals	
MPA	SI	Megapascals	
ATMG		Atmospheres, gauge	
MMH2OG		Millimeters of water, gauge	
INH2OG		Inches of water, gauge	
BARG		Bar, gauge	
DY/CM2G		Dynes per square centimeter, gauge	
G/CM2G		Grams per square centimeter, gauge	
KG/CM2G		Kilograms per square centimeter, gauge	
KG/M2G		Kilograms per square meter, gauge	
KPAG		Kilopascals, gauge	
MPAG		Megapascals, gauge	
PAG		Pascals, gauge	

**NOTE:** Standard conditions are:

STP	60 F	14.696 PSIA
NTP	0 C	1 ATM
API	15 C	1 ATM

## Output Units: By System

**NOTE:** For engineering convenience, Design II uses KPA and KJ as SI units rather than the strict SI standard units, pascals and joules.

<u>Quantity</u>	<u>Default</u>	<u>SI Units</u>	<u>Metric Units</u>
Quantity	LBMOL	KGMOL	KGMOL
Time	HR	SEC	HR
Temperature	F	K	C
Pressure	PSIA	KPA/MPA	KG/CM2
Enthalpy	BTU	KJ	KCAL
Entropy	BTU/LBMOL/R	KJ/KGMOL/K	KCAL/KGMOL/K
Density	LB/FT3	KG/M3	KG/M3
Surface Tension	DYNE/CM	DYNE/CM	DYNE/CM
Length	FT	M	M
Heat Capacity	BTU/LBMOL/R	KJ/KGMOL/K	KCAL/KGMOL/C
Viscosity	CP	NS/M2	CP
Thermal Conductivity	BTU/FT/HR/F	W/M/K	KCAL/M/HR/C
Power	HP	WAtts	HP
Heat Transfer	BTU/HR/FT2/F	KJ/SEC/M2/K	KCAL/HR/M2/C
<b>Stream Summary</b>			
NTP or STP liquid	GAL/MIN	M3/HR	M3/HR
NTP or STP vapor	MMSCFD	M3/HR	M3/HR
Component flowrates	LBMOL/HR	KGMOL/HR	
<b>Stream Details</b>			
T-P liquid	GAL/MIN	M3/HR	M3/HR
T-P vapor	FT3/SEC	M3/HR	M3/HR
NTP or STP liquid	S.G.(60/60)GPA	M3/HR	
NTP or STP vapor	MMSCFD	M3/HR	M3/HR
Component molar flowrates (liquid & vapor)	LBMOL/HR	KGMOL/SEC	KGMOL/HR
Dew point vapor or bubble point liquid	Mole %	Mole %	Mole %
Component mass flowrate	LB/HR	KG/SEC	KG/HR

**NOTE:** Standard conditions are:

STP	60 F	14.696 PSIA
NTP	0 C	1 ATM

# Chapter 12

---

API

15 C

1 ATM

# Chapter 13: Stream Files

These commands should be used only when specifications for a large number of streams will have to be retrieved for subsequent runs. Filenames can be short or long.

**NEW STR**eam file = *name*

Used to create a stream file to store TP and FLO data for streams listed on SAV STR command.

**SAVe STR**eams = *j, ...*

Enter stream number of streams for which you want TP and FLO data stored in the stream file. Streams must be in ascending order.

**OLD STR**eam file = *name*

Enter the name of the existing stream file to be accessed.

**REAd STR**eams = *j, ...*

Enter stream numbers of streams for which you wish to retrieve data from an OLD STR file.

**ERAsE STR**eam file = *name*

Enter the name of the existing stream file when you want it to be erased.

**NOTES:**

1. Only one stream file can be accessed in a single run.
2. Crude streams cannot be saved (SAV STR=) and read (REA STR=) without some special care. This is because only the pseudo component ID number and flow rate are saved, not the pseudo component temperature, specific gravity, and molecular weight properties. Therefore in reading the saved crude stream, it is necessary to insure that the pseudo components in the "reading run" are exactly identical to those in the "saving run". This can be accomplished by allowing Design II to create them in the same manner in both runs or by explicitly defining the pseudo components (with CUT=, FEE COM GRA=, and FEE COM MOL=).

## Stream Files Step by Step

**Choose commands listed below for use with a Stream data file**

Create a stream file

**NEW STR** = *name*

Save stream data in a stream file

**SAV STR** = *j,..*

Access an existing stream file

**OLD STR** = *name*

Read data from a stream file

**REA STR** = *j,..*

Erase existing stream file

**ERA STR** = *name*

**NOTE:** The filename for a Stream file can be short or long. Only one stream file can be accessed in a single run.



# Chapter 14: Saving Stream Data

For flowsheets with many feeds and recycles or flowsheets that need to be broken down into sections, it is often useful to save data for some streams to be used in the next run. Only feed or recycle guesses need to be saved, not all streams.

## Example:

To save stream temperature, pressure and component flowrates for streams 1,5,8 and 13 the commands entered in the GENERAL section would be:

**NEW STR** = RECTISOL.DAT

**SAV STR** = 1,5,8,13

To access the streams on the next run, the following commands would be entered:

**OLD STR** = RECTISOL.DAT

**REA STR** = 1,5,8,13

To read in streams and then write data for the same or different streams into the existing file enter:

**OLD STR** = RECTISOL.DAT

**REA STR** = 1,4,10

**SAV STR** = 2,4,15

**NOTE:** An old file can be erased in the same run the stream information is being read. A new file cannot be written at the same time a file is being erased.

Only one stream file can be accessed in a single run.

## Refine module REStart files

The solution of the nonlinear algebraic equations for a REFIne column is stored in a restart file and subsequent runs of the REFIne column can read this file and restart their calculations from the column's previous solution. This can reduce runtime by more than 50%.

**NEW REStart** FIL = filename

Create a new restart file

**OLD REStart** FIL = filename

REad or write to an existing restart file

The filename for a Restart file can be short or long. Only one Refine Restart file can be accessed in a single run.





# Chapter 15: Case Study

The CASE Study section allows an engineer to run a number of similar simulation cases at once in order to assess the sensitivity of a flowsheet to changes in variables or to produce a number of design cases. CASE study allow you to present your results in data tables and plots for efficient analysis. This has the effect of reducing both the engineering and computer time required.

There is a limit of 1000 cases that may be specified in one CASE study and only one CASE study section per flowsheet. All parameter changes will be implemented and the entire flowsheet is recalculated with the new parameter setting.

## Case Study Command Details

### Equipment Name (All Are Required)

#### CASE study

This command is required to begin the CASE study section of the input and is used only once per flowsheet.

#### CASE block

The CASE block command marks the beginning of a new input case. Each CASE block may specify any number of flowsheet parameter changes. All parameter changes will be implemented and the entire flowsheet is recalculated with the new parameter setting. There is a limit of 1000 cases that may be specified in one CASE study. NAME = - up to 16 characters The name command labels each CASE block.

**NOTE:** The Case Study section MUST be the last section in the input. The only exception is that the FORTRAN library, if present, must follow the CASE study section. Only one Case Study is allowed.

#### CHANGE, module/stream nnn,parameter (units) =value, RESTore

The CHANGE command is used to modify the value of a parameter in the flowsheet. A list of valid parameters is given in Tables 2 and 3 of the Inline FORTRAN section. 'nnn' refers to the equipment module or stream number.

The CHANGE command may optionally be followed by the RESTore keyword. This has the effect of restoring the parameter value to its original value after the current case is completed.

#### STEP, module/stream nnn, parameter (units) = value, INCrement = , LIMit=, RESTore

The STEP command is a convenient way to specify a series of cases where a parameter is being varied in a systematic fashion. This generates a set of cases, with the parameter being incremented by the amount specified for each successive case until the specified limit is exceeded. This is equivalent to a series of CHANGE commands. A list of valid parameters is given in Tables 2 and 3 of the *Inline FORTRAN* section. 'nnn' refers to the equipment module or stream number.

The STEP command may optionally be followed by the RESTore keyword. This has the effect of restoring the parameter value to its original value after the current case is completed. If the increment is negative, the limit becomes a lower limit. There is a limit of 500 cases that may be run with a single STEP command.

**NOTE:** Only one STEP command per CASE block is allowed. CHANGE commands may be used in the same CASE block as the STEP command and will be in effect for each increment of the STEP command. Care should be taken not to CHANGE the same parameters that are in the STEP command to minimize conflict.

### Control Output

#### Choose one or more of the following:

#### TABLE, module/stream nnn, parameter, LABEL=

The TABLE command allows you to build a comparative table for case studies. All variables which occur in CHANGE or STEP statements will automatically be reported in the table. The user may add to this list by using the TABLE command. The list of valid parameters is identical to the parameters available to Inline FORTRAN and are called using the same keywords that are used by *Inline FORTRAN* (Tables 2 and 3).

It is possible to use the TABLE command if no CASE blocks are specified. This is an easy way to get a compact summary of key variables.

#### PLOTX, module/stream nnn, parameter, LABEL

and

#### PLOTY, module/stream nnn, parameter, LABEL

The PLOTX/PLOTY commands allow you to graph the changes in one variable against another. The PLOTX command defines the independent variable and the PLOTY defines the dependent variable. UP to four dependent variables (PLOTY) may be defined on the same graph if each has the same dimensional units. the same parameters are available to the PLOT command as are available to the TABLE command. The LABEL may be up to 16 alphanumeric characters. Multiple graphs may be defined by additional PLOTX/PLOTY commands.

## Case Study Format Section

Case study commands are entered in the DESIGN II input file in accordance with the following guidelines.

## Chapter 15

1. text
2. text
- .....
- 10 text

CASe studies, by their nature, tend to produce extremely large output files. Unless the detailed information is required, use the GENeral section, PRInt SWItch = 3 and PRInt STReam - NONE options to reduce the volume of output.

There is an overall limit of 1000 cases that may be specified in one run. There will normally be one case per CASe block; however, if a STEp command is used, a CASe is run for each increment. A maximum of 500 cases may be generated by one STEp command. This is to prevent a poor specification from effectively causing an infinite log.

CASe study uses the converged solution from one calculation as the starting point for the next. Because of this, it is advantageous to arrange the case studies in such a way that the step (or change) from one case to the next is as small as possible. This will both reduce the amount of computer time required and increase the likelihood of convergence.

1. The primary keywords CASeblock, CHAnge, STEp, and TABLe must begin a new line.
2. Variables are coded in the same way as in the standard input with the exception of multiple value variables. To refer to a particular value of a multiple value variable, it is necessary to refer to the value's position. For example, the third stage of a multi-stage compressor is specified with the syntax PRE STA 3.
3. The CASe study section must be the last section in the input. The only exception is that the FORTRAN library may follow the CASe study section.
4. Only one CASe study section is allowed. You may use multiple CASe blocks in one CASe study.
5. Comment lines, beginning with 'C-' may appear anywhere within the section.
6. No Inline FORTRAN is allowed in the section.
7. Commands may be spread over multiple lines. A new line may begin wherever a comma would be inserted. A line may not begin with an equipment module identifier.
8. When generating multiple plots, the dependent variables (y) will be grouped with the appropriate independent variable (x) as they are sequentially listed in the input file. When a PLOTX variable is specified, all subsequent PLOTY variables will appear on the same plot until another PLOTX command appears. See following examples.
9. The variables which are changed in the CASe study section must be specified in the input and should not be calculated or derived quantities, since the change will be lost when such quantity is recalculated.
10. Characters shown in CAPitals are the minimum recognizable KEYWORDS which must be entered in this section.

### Case Study Examples

#### Example of CHAnge command:

```
CHANGE, COMPRESSOR 5, PRESSURE OUT = 200, RESTORE
```

#### Example of STEp command

```
STEP, COMPRE 5, PRE OUT (PSIA)=200, INC=20, LIM=300, RESTORE
```

#### Example of TABLe command:

This example shows the use of the TABLe command without a CASe block. This is an efficient way to get a compact summary of key variables.

#### CASe study

```
TABLE, COMPRE 5, CALCULATED WORK, LABEL=K101 WORK
```

#### Example of PLOTX/PLOTY commands

```
CASe study CASe block,  
NAME=EXAMPLE3  
PLOTX,COMPRE 5, PRESSURE OUT, LABEL=K101 PRESSURE OUT PLOTY,COMPRE 5, CALCULATED WORK, LABEL=K101 WORK  
PLOTX, STREAM 7, FLO, LABEL = PURGE RATE PLOTY, STREAM 7, FLOW COMPONENT 4, LABEL=METHANE LOSS  
PLOTY,STREAM 7, FLOW COMPONENT 5, LABEL = ETHYLENE LOSS
```

Two complete sample input files follow. The table and plots from the condensing curve (FLAsh) case study are also included.

### Case Study Samples

There are several sample flowsheets in "Chapter 5: Case Study Samples - c:\designii\samples\casestdy" of the DESIGN II for Windows Tutorial and Samples Guide.

# Chapter 16: ChemTran

## ChemTran Overview

Accurate physical property and thermodynamic data are essential for a process simulator to provide accurate process design, equipment sizing, energy balance, and mass balance of calculations. ChemTran provides the ability to define, regress, and predict all thermophysical properties necessary for accurate process simulation calculations. ChemTran is designed to integrate experimental data and physical property prediction methods with DESIGN II data correlations to improve their accuracy and increase their applicability. In many applications it is not necessary to use ChemTran to accurately model a process with DESIGN II. However, ChemTran may be required to augment DESIGN II's physical property database and thermodynamic correlations when modeling processes involving non ideal chemical systems, proprietary chemical components, or extreme process conditions.

---

## ChemTran: Applications

---

DESIGN II already contains all thermodynamic and physical properties necessary to accurately model many chemical systems. DESIGN II's database contains thermophysical properties for over 886 components and includes over 100 thermodynamic correlations. There are occasions however when the DESIGN II database should be supplemented or modified in order to obtain the most accurate simulation. Situations where ChemTran may be required are listed below:

### **Enter physical property data for a component not present in DESIGN II's database.**

Use ChemTran's extensive group contribution physical property estimation methods to predict thermodynamic and physical property for user defined components when experimental or literature data is unavailable.

### **Enter physical properties found in the literature or determined experimentally.**

In some circumstances it may be desired to base the process simulation on physical properties other than those contained in the DESIGN II database. ChemTran allows the flexibility to override the standard database properties and enter properties obtained from another source.

### **Enter thermodynamic data for non ideal systems.**

When Chemical systems have strong intermolecular interactions, are difficult to separate, or have strong heats of solution, it is necessary to enter data that accounts for non ideal behavior. ChemTran provides the capability to regress thermodynamic data, enter interaction parameters, or enter infinite dilution activity coefficients to account for non ideal chemical systems. Use UNIFAC or regular solution theory to predict infinite dilution activity coefficients where experimental phase equilibrium data is scarce.

---

## ChemTran: Database List

---

ChemTran contains the same physical property database that is included in DESIGN II. This database includes physical properties for over 1235+ chemical components. ChemTran provides access to the database to permit the user to create his own data file that includes additions and modifications to the physical property database. A complete list of the components is found in *Component Database Sorted By ID*

---

## ChemTran: Pure Component Physical Property Entry, Regression and Estimation

---

ChemTran provides capability to enter, regress, or estimate pure component physical property data. These properties are stored in a user defined database and is used to supplement the DESIGN II standard pure component physical property database. ChemTran provides the ability to enter the following pure component point properties:

Normal Boiling Point	Critical Temperature	Critical Pressure
Critical Volume	Molecular Weight	Component Name
Acentric Factor	Solubility Parameter	

Additionally, ChemTran provides the ability to regress the following temperature dependent properties.

Ideal Gas Heat Capacity	Latent Heat	Vapor Pressure
Surface Tension	Density	Viscosity
Thermal Conductivity	Enthalpy	K-Values

ChemTran provides group contribution methods to estimate the following physical properties. The user only needs to enter the molecular structure of the component and ChemTran determines what relevant groups are present and calculates their contribution for each physical property.

Normal Boiling Point	Critical Temperature	Critical Pressure
Critical Volume	Component Name	Acentric Factor
Solubility Parameter	Surface Tension	Ideal Gas Heat Capacity
Viscosity	Vapor Pressure	Enthalpy
Density	Thermal Conductivity	

---

### ChemTran: Mixture Data Entry

---

Chemical mixtures having strong intermolecular interactions will exhibit non ideal equilibrium behavior and therefore it is necessary to include binary interaction parameters in the thermodynamic correlation to accurately predict the mixture's VLE or LLE behavior. ChemTran provides the following methods for determining the Binary interaction parameters.

- Regressing Experimental or Literature. See *ChemTran: Phase Equilibria Data*
- Entering Binary Interaction Parameters (BIP's). See *ChemTran: Mixture Command Details*
- Entering *ChemTran: Activity Coefficients at Infinite Dilution*
- Estimating Infinite Dilution Activity Coefficients from the UNIFAC group contribution method or Regular Solution Theory. See *ChemTran: Mixture Command Details*

Interaction parameters can be correlated for the following *ChemTran: K-Value Options*.

Peng-Robinson	Modified Peng-Robinson
Soave	API Soave
Renon (NRTL)	Wilson
UNIQUAC	

---

### ChemTran: When to Use ChemTran

---

ChemTran should be used for:

- entering pure component physical property data.
- entering pure component tabular data.
- generation of pure component data from bond contributions.
- correlation of VLE and LLE data, excess enthalpy data.

It is necessary to use ChemTran when component data is not contained in the PURE COMPONENT DATABASE or cannot be entered directly into DESIGN II.

A file containing physical property data, correlated equations for tabular data, and interaction constants from reduction of vapor-liquid or liquid-liquid equilibrium (VLE or LLE) data can be created in ChemTran. DESIGN II gains access to this data via a CHEMtran FILE command found below.

#### **CHEMtran FILE command.**

The file names (3 sets of 4 characters separated by commas) used in DESIGN II must be the same names used in ChemTran when the file was created. The COMponents command used for the DESIGN II run does not have to match the COMponents command used in the ChemTran run. For details on creation of CHEMtran FILES, refer to *ChemTran File Access Commands*.

The following K-value options are typically used for VLE data regression: RENon, UNIQUACK, WILson, APISOAVEK, SOAVEK and PENK. Be sure to specify the appropriate K-value option in the GENERAL section if your CHEMtran FILE contains results of VLE (or LLE) data regression.

Error messages will print after the ECHO PRINT OF INPUT DATA if the file is either not found or an incorrect password (the third name on the CHE FIL command) has been specified. Take appropriate steps to correct the problem.

- 1) Rerun ChemTran to recreate the file or
- 2) Correct spelling of the file names.

DESIGN II output shows the dates the CHEMtran FILE was created and last modified. Check to be sure these dates match those shown in your ChemTran output.

---

### ChemTran: Executing ChemTran

---

ChemTran contains a complete set of easy to use keyword commands that allow the user to add to or modify the pure component physical property database or thermodynamic correlations. The keywords are entered into an:

INPUT FILE which MUST

- have your account number on the first line
- have a DOS filename and be an ASCII file with the extension \*.IN
- be prepared with an Windows Input Manager (Under Simulate...ChemTran)
- be in UPPER CASE CHARACTERS ONLY
- not contain any TABS
- have CONTINUING lines indented 5 spaces.

ChemTran can be executed in a batch mode for example, by typing: C386 filename (no extension) then press ENTER.

ChemTran creates two output files.

1. The first output file is an ASCII text file and is intended for evaluation by the user to determine if the second file was correctly executed and prepared.
2. The second output file is called the CHEMical FILE which is accessed by DESIGN II.

A step by step example of how to build your ChemTran input file is shown in *ChemTran Example Input File*

---

## ChemTran: Global Output Unit Specification

---

The method for specifying output units is to select an overall units system to be used for **ALL** output. These commands change all output units to the specified system. The commands to use before the END statement for selecting this method are:

### AMERICAN UNITS OUT

Specifies American or US units system for all output.

### SI UNITS OUT

Specifies SI units system for all output.

### METRIC UNITS OUT

Specifies metric units system for all output.

### Example 1.

If you want all output data reported in the standard SI units, enter the command:

### SI UNI OUT

---

## ChemTran: Example Input File

---

The following ChemTran Input File can be coded under the DESIGN II option , Simulate ...Use ChemTran...Input Manager Window.

```

AB123.
*   Introducing 2,4-dichlorotoluene as Component 200 and Regressing
C-  Acetone-Water Data.

C-  Note that a comment may be added by beginning the line with C-.

COM =          200,          1002,          62
C-   2,4-dichlorotoluene,  Acetone,  Water

C-  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
C-  PURE COMPONENT PROPERTIES.
C-  The STRUCTURE command alone would generate properties for the new
C-  component, but additional data has been input for purposes of illustration.
C-  ChemTran inserts hydrogen atoms to fulfill valence requirements.

STRUC 200 = C1-C2, C2=C3, C3-C4, C4=C5, C5-C6, C6=C1, C2-CL7,
        C4-CL8,C1-C9
NAME   200 = DICHLOROTOLUENE
TB (F) 200 = 405.29
TC (F) 200 = 826.34
PC (PSIA) 200 = 521.12
VC (FT3/LBMOL) 200 = 6.5996
CP-T (BTU/LBMOL/R,K) 200 = 47.780,500,47.780,510

C-  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
C-  MIXTURE PROPERTIES.
C-  VLE data for Acetone-Water. Reference: Verhoeye, De Schepper,
C-  J. Appl. Chem. Biotechnol. 23, 607(1973).

T-X-Y (MMHG,C) 1002,62 = 760,
    76.25,    .0490,    .6050,
    72.40,    .0690,    .6780,
    66.45,    .1270,    .7530,
    62.75,    .2000,    .7900,
    62.34,    .2760,    .8040,
    60.90,    .4000,    .8260,
    60.17,    .4950,    .8320,
    58.80,    .6500,    .8550,
    58.47,    .6940,    .8620,
    57.95,    .7500,    .8760,
    57.25,    .8290,    .9030,
    56.75,    .9000,    .9360,
    56.45,    .9400,    .9590,

WILSON
FILE NEW = EXAM,PLE,DATA
PRINT PROPERTIES
END

```

## ChemTran Files and Data Libraries

ChemTran Files is a powerful tool that can increase your productivity by automating the prediction and correlation of thermophysical properties for chemicals. DESIGN II has a built-in data base of pure component properties and mixture correlations to model many types of processes without additional property data. When this additional data is necessary, ChemTran is the only program you will ever need to furnish all the properties required by DESIGN II for performing heat and material balance calculations. ChemTran is an ideal tool for handling properties for non-ideal chemical systems or hydrocarbon systems where unusual properties must be taken into account.

A file containing physical property data, correlated equations for tabular data, and interaction constants from reduction of phase equilibrium data can be created in ChemTran and used when component data is not contained in the PURE COMPONENT DATA BASE or cannot be entered directly into DESIGN II.

The ChemTran program is used for:

- Entering pure component physical property data.
- Entering pure component tabular data.
- Generation of pure component data from bond contributions.
- Entering ionic component data and reaction descriptions.
- Correlation of multicomponent V-L-E, L-L-E, L-L-L-E, V-L-L-E data, and excess enthalpy data.
- Regression of binary, ternary, quaternary, etc. data simultaneously to liquid activity coefficient equations or to equations of state.

The component list for DESIGN II does not have to match the one used in ChemTran to create the library data file. Missing property information will be supplied from our pure component data base.

Be sure to specify the same K-value and enthalpy options in the GENERAL section that you used in the ChemTran run if you were regressing vapor-liquid or liquid-liquid equilibrium data or excess enthalpy data.

**NOTE:** Only one CHEmtran FILE can be accessed per simulation.

DESIGN II gains access to this data via a CHEmtran FILE command. The file names used in DESIGN II must be the same names used in ChemTran when the file was created.

**CHEmtran FILE** = name1,name2,name3

Enter the 3 names of your ChemTran data file which is to be read by DESIGN II. "name1", "name2", and "name3" may only be 1 to 4 characters in length. This file is used to store user-provided thermodynamic data and/or physical property data. See sections 1 and 2 of the ChemTran manual for commands and guidelines for creating the CHEmtran FILE.

**Example: CHE FIL = MEOH,MTBE,DATA**

DESIGN II also has several libraries of binary interaction parameters obtained from regression of equilibrium data (typically vapor-liquid equilibrium data) which you can use. A binary interaction library is automatically loaded when you select the Lee-Kesler-Ploecker equation option (LKPK). You may use either or both of the following libraries with the Peng-Robinson equation option (PENK).

**BINARY PARAMETERS = PENG1.**

Peng-Robinson; Binary Interaction Parameters. The PENG1 data file will only be used with the Peng-Robinson equation of state (PENK). It contains binary interaction parameters for the components listed in *Table 3*.

**PETroleum BINARY PARAMETER = GPA1**

The Peng-Robinson binary parameter library includes petroleum fraction interactions. The Gas Processors Association has suggested binary parameters for petroleum fractions interacting with the components shown below.

Petroleum Fraction Interactions	C1 - petroleum fraction
N2 - petroleum fraction	C2 - petroleum fraction
CO2 - petroleum fraction	C3 - petroleum fraction
H2S - petroleum fraction	petroleum fraction - petroleum fraction

These parameters improve the accuracy of the Peng-Robinson (PENK) correlation for mixtures which contain components numbered between 100 and 199 (petroleum fractions or CRUde feed section).

The following interaction parameter tables are based on the UNIFAC group contribution technique and match regressed VLE or LLE data reasonably well. Both VLE and LLE parameter tables can be requested in the same simulation.

**LLE UNIFAC = 1**

The LLE Unifac parameter library group interactions available for 32 different groups including hydrocarbons, water, alcohols, organic acids, and other compounds. This option should be used in conjunction with the LL UNIFACK choice. Reference 20g.

**VLE UNIFAC = 2**

(Default) The VLE Unifac parameter library group interactions available for 44 different groups including hydrocarbons, water, alcohols, organic acids, and other compounds. This contains the fourth revision and extension of UNIFAC parameters by Rasmussen, et al. This option should be used in conjunction with the UNIFACK choice. Reference 20f.

**VLE UNIFAC = 1**

The VLE Unifac parameter library group interactions. This contains the original UNIFAC parameters and the first through third revisions and extensions. This option should be used in conjunction with the UNIFACK choice. References 20a-e

**ChemTran Modified Peng-Robinson Example Input**

The following example shows how ChemTran is used to regress **CO<sub>2</sub>-water** VLE data to the modified Peng-Robinson method.

AB123.

\* CHEMTRAN input file to be used with DESIGN II input file.

C- Water, CO<sub>2</sub>

COMPONENTS = 62, 49

C- Specify MODified PENg Robinson equation of state with MARGules mixing rule.

**MODPENK (MARGULES)**

C- Specify regression of Kappa parameters from library

C- vapor pressure data KMODPEN (VAPOR) 62

**KMODPEN (VAPOR) 49**

C- Regress VLE data

**P-X-Y (BAR,K) 49,62 = 383.15,**  
 99.999,.0140,.9560,  
 199.997,.0210,.9580,  
 299.995,.0240,.9480,  
 399.994,.0260,.9320,  
 499.992,.0280,.9140,  
 599.991,.0300,.8930,  
 699.990,.0315,.8720,  
 799.988,.0330,.8540,  
 899.986,.0345,.8400,  
 1499.997,.0400,.8000,

**P-X-Y (BAR,K) 49,62 = 423.15,**  
 99.999,.0135,.8800,  
 199.997,.0215,.9100,  
 299.995,.0260,.9000,  
 399.994,.0290,.8820,  
 499.992,.0320,.8620,  
 599.991,.0345,.8400,  
 1499.997,.0480,.7520,

**P-X-Y (BAR,K) 49,62 = 473.15,**  
 99.999,.0130,.7150,  
 199.997,.0260,.8200,  
 299.995,.0340,.8250,  
 399.994,.0410,.8160,  
 499.992,.0470,.8000,  
 599.991,.0520,.7800,  
 999.985,.0630,.7200,

**P-X-Y (BAR,K) 49,62 = 543.15,**  
 599.991,.1060,.5460,  
 699.990,.1250,.5200,  
 799.988,.1450,.4960,  
 899.986,.1660,.4620,  
 1299.982,.2880,.2880

END

## ChemTran Entering Data

When dealing with component mixtures that interact non-ideally (homogeneous or heterogeneous azeotropes, highly-polar components, liquid-liquid, etc.), DESIGN II needs information which will describe the degree of non-ideality between the various components in your system. The best description can be provided with measured vapor-liquid or liquid-liquid (VLE or LLE) equilibrium data. The DESIGN II PURE COMPONENT DATA BASE only has pure component property data stored, **not VLE data**.

**NOTE:** For non-standard components (ID numbers 200-299), the critical properties, boiling points and acentric factors that you enter (or the program estimates) are very important in the calculation of K-values, particularly for the equation-of-state techniques.

## ChemTran File Access Commands

The following commands should be employed to store the results of a ChemTran run on a non database pure component property generation or on a VLE/LLE data regression. These results will be accessed by DESIGN II for simulation. See *ChemTran-DESIGN II Interface* for sample illustration of this command.

### File Creation

**FILE NEW** = name 1, name 2, name 3

This command tells ChemTran to create a new data file and store property data. The properties may consist of a combination of pure component and multicomponent data. Labels are attached to the file through the variables name1,name2,name3.

## Chapter 16

Each of these parameters is a name consisting of one to four characters. This command may be inserted at any position between the title and END command. The file so created will exist under the directory as *name1name2.name3*.

### File Usage, Maintenance, and Deletion

**FILE OLD** = name 1, name 2, name 3, key

This command provides for the usage and/or deletion of a private data file created in a previous execution of ChemTran. The parameters name1,name2,name3 consist of one to four characters and must be the same as the ones used for the creation of the file with a FILE NEW command. Values for the key parameter are

<b>KEY</b>	<b>Operation Performed by ChemTran</b>
0	reads an old file
2	reads an old file, then erases it; creates and writes a new file
3	writes on an old file
4	erases an existing file; before submitting for execution. Remove from your input all commands that enter VLE data

As with the FILE NEW command, the FILE OLD statement may be placed at any point between a Title and END command.

**NOTE:** Only one file can be accessed per run

## ChemTran DESIGN II Interface

This command is used only when DESIGN II will be retrieving data from a ChemTran run. This data typically results from correlation and/or prediction of vapor-liquid equilibrium data and pure component data for non- standard components (ID numbers 200-299). File names must contain a legal file name for the platform that DESIGN II / ChemTran is running on.

**CHEmtran FILE** = *name*

Enter the name of your ChemTran data file to be accessed by DESIGN II.

### NOTES:

1. Only one CHEmtran FILE can be accessed in a single run.
2. IBM systems also require a change in the job control language (JCL) for file FT36F001.

Contact your Computer Support Group for more information.

A sample output showing CHE FIL access by DESIGN II is shown below.

```
ECHO PRINT OF INPUT DATA

*THREE PHASE FLASH
MULTIPLE PHASE FLASH 1 = VOL,1,-2,-3,-4 GENERAL,
      COMPONENT = 1,1021,62,41,3
      FLOW 1 = 50,5,20,25,0
      TP(C)1 = 25,14.7
      RENON, LATENT HEAT
      CHEMICAL FILE = TOLU,MEOH,DATA

END

THERMO DATA FILE OPENED FOR READ
CHEMICAL FILE ACCESSED WAS CREATED 05MAY96 10:32:01
AND LAST MODIFIED 05MAY96 10:32:01
NUMBER OF COMPONENTS ON FILE = 3
      1021 METHANOL
      62 WATER
      41 TOLUENE
```

### Related Sample ChemTran Input File

```
AB123.
*TOLUENE/ WATER/METHANOL DECHEMA DATA
C-
C- LIQUID-LIQUID EQUILIBRIUM DATA
C- TOLUENE WATER METHANOL

COMPONENTS = 41, 62, 1021

C- AUTHOR -

C- TEMP. UNITS: DEGREES C CONC. UNITS: MOLE FRACTION
C- PRESSURE = 760 MMHG

T-X-Y (MMHG, C) 41,62,1021 = 760,

C- (1) TOLUENE C7H8
```



```

C- (2) WATER H2O
C- (3) METHANOL CH4O

C-TEMP. LIQUID LIQUID VAPOR VAPOR
C- PHASE PHASE PHASE PHASE
C- C CONC(1) CONC(2) CONC(1) CONC(2)

77.25, .1111, .5555, .5555, .1111
...
Please enter the appropriate data
...
79.80, .9999, .0001, .0001, .9999

```

RENON { (or) WILSON (or) UNIFAC K---Please Choose **ONLY ONE THERMO**}

FILE NEW=TOLU,MEOH,DATA

PRINT PROPERTIES

## ChemTran Electrolyte (Ionic) Component Data Entry

DESIGN II has implemented the Edwards et al. method for weak aqueous electrolytes. This method requires many thermophysical properties for the components and ions present in the solution. ChemTran and DESIGN II data banks include all required thermophysical data for sour water applications.

Applications of electrolytes should be restricted to the following conditions:

- The solvent must be water only
- Total solute concentrations should be 10 molal
- Ionic strength should be 6 molal
- Henry's constants must be available for all solutes
- Mixed solvents and crudes are not supported
- User defined reactions should be in mass and charge balance
- No strong electrolytes or salts are allowed
- Transport/Physical properties are not corrected for ionic effects

Electrolyte Thermodynamics require ChemTran when the electrolyte system being modeled includes ions, reactions, and solutes not present in the DESIGN II databanks shown below:

---

### ChemTran: Electrolyte Component Theory

---

DESIGN II and ChemTran provide new electrolyte thermodynamics which will extend the range of chemical systems which can be simulated. Electrolytes solutions differ from other solutions because of the presence of ions created by dissociation reactions. A weak electrolyte is distinguished from a strong electrolyte in that it does not dissociate completely. Ammonia in water is an example of a weak aqueous electrolyte solution.

Electrolyte solutions differ from non-electrolyte solutions primarily due to the presence of ions and the long range electrostatic forces between those ions. For this reason, thermodynamic correlations that do not account for these forces do not predict electrolyte system phase equilibria accurately.

Peter Debye and Erich Huckel derived a model which accounts for these electrostatic forces in 1923 (2). Their work is the basis for many models developed since then.

DESIGN II supports an equilibrium model for weak, aqueous electrolytes based on modifications by Edwards, Maurer, Newman and Prausnitz to an extended Debye-Huckel model, as published in the AIChE Journal, 1978 (1).

This model accounts for ionic reactions in liquid phase and therefore requires all ionic species and reactions be defined along with the associated ionic reaction equilibrium constants. In addition, Henry's law constants are required to calculate solute liquid phase concentrations. This model is combined with the Redlich - Kwong equation to determine vapor phase fugacity coefficients.

---

### ChemTran: Electrolyte Component Library

---

<u>Ion ID Number</u>	<u>Ion</u>
9401	H+
9402	OH-
9631	S=
9632	HS-
9633	SO3-
9634	HSO3-
9651	CO3=
9652	HC03-
9661	CN-
9701	NH4+

## Chapter 16

9711

NH<sub>2</sub>COO<sup>-</sup>

---

### ChemTran: Ionic Reaction Library

---

#### Library Reactions for Ionic Compounds

1-99 User-defined reactions  
100+ Design II provided Reactions

<u>Ionic Reaction ID</u>	<u>Ionic Reaction</u>
101	H <sub>2</sub> O <-> H <sup>+</sup> + OH <sup>-</sup>
102	CO <sub>2</sub> + H <sub>2</sub> O <-> H <sup>+</sup> + HCO <sub>3</sub> <sup>-</sup>
103	HCO <sub>3</sub> <sup>-</sup> <-> H <sup>+</sup> + CO <sub>3</sub> <sup>=</sup>
104	H <sub>2</sub> S <-> H <sup>+</sup> + HS <sup>-</sup>
105	HS <sup>-</sup> <-> H <sup>+</sup> + S <sup>-</sup>
106	SO <sub>2</sub> + H <sub>2</sub> O <-> H <sup>+</sup> + HSO <sub>3</sub> <sup>-</sup>
107	HSO <sub>3</sub> <sup>-</sup> <-> H <sup>+</sup> + SO <sub>3</sub> <sup>=</sup>
108	HCN <-> H <sup>+</sup> + CN <sup>-</sup>
109	NH <sub>3</sub> + H <sub>2</sub> O <-> NH <sub>4</sub> <sup>+</sup> + OH <sup>-</sup>
110	NH <sub>3</sub> + HCV <sub>3</sub> <sup>-</sup> <-> NH <sub>2</sub> COO <sup>-</sup> + H <sub>2</sub> O

**NOTE:** These reactions may be combined to specify other reactions. E.g. NH<sub>3</sub> + CO<sub>2</sub> + H<sub>2</sub>O <-> NH<sub>4</sub><sup>+</sup> + HCO<sub>3</sub><sup>-</sup>. This is a combination of reactions 102 + 109 - 101.

---

### ChemTran: Electrolyte System Data

---

Information which is necessary for using the electrolyte model falls into four primary groups: ion information, ionic reaction information, Henry's constant information and model binary interaction parameters.

#### i) Ionic information

Ionic formula and charge are required. Refer to *ChemTran: Electrolyte Component Library* for ions present in the ion component library. For ionic species not present in the component library, data must be entered using ChemTran.

#### ii) Ionic reaction

Information ionic reaction stoichiometry and equilibrium constants are required for each reaction occurring. If ionic reactions are occurring that are not listed in *ChemTran: Ionic Reaction Library*, then ChemTran should be used to enter the reaction stoichiometry and equilibrium constants. ChemTran does not provide regression capabilities to calculate equilibrium constants from equilibrium data.

#### iii) Henry's constants

Henry's constants are required for all solutes in water. The components for which Henry's constants are available in DESIGN II are listed in *Thermodynamics: Table 5. Henry's Constants in Water List*. Henry's constants for other components must be entered with ChemTran.

#### iv) Model interaction parameters

Binary interaction parameters for ion-ion, molecule-ion, molecule-molecule pairs should be specified. The DESIGN II data banks include all interaction parameters required to model the ionic reactions listed in *ChemTran: Ionic Reaction Library*. If other ionic species or ionic reactions are present, ChemTran will be used to enter interaction parameters. Without these parameters, the model reverts to an extended Debye-Huckel model which will be valid for items of ionic strengths of 0.1 molal or less. ChemTran does not provide regression capabilities to calculate interaction parameters from equilibrium data.

---

### ChemTran: Electrolyte Command Details

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If you determine that ChemTran is required, follow the keyword instructions discussed below on using ChemTran to enter the required data.

#### EDWARDK

This keyword selects the Edwards method for weak aqueous electrolytes

**ION COMPONENTS** = 9401,...,9999 Enter ionic component ID numbers. Component numbers 9401-9899 are reserved for library components. Components numbers 9900-9999 are reserved for user defined ionic components.

**ION NAME** i = Enter the desired name for the ion. ION NAME 9901 = H<sub>2</sub>PO<sub>4</sub><sup>-</sup>

**ION FORMULA** i = # of atom1 \* atom1, # of atom2 \* atom2,...  
Where i = ion ID number. Number must be in the 9900's.

This command is required to define all ionic species that are not in the Ion Component Library.

Example: The ion (H<sub>2</sub>PO<sub>4</sub><sup>-</sup>) would be entered as:

**ION FOR** 9901=2\*H, 1\*P, 4\*O

**NOTE:** This command must be used in conjunction with **IONIC CHARGE** command seen below.

**IONIC CHARGE** i = value

Enter ionic charge. H<sub>2</sub>PO<sub>4</sub><sup>-</sup> has an ionic charge of -1 which is entered as follows:

**ION CHA** 9901= -1

**LIBRARY REACTION** = 101,101,...1,2,...

Enter reaction ID numbers. 100+ are reserved for library reactions. These reactions will have database information for stoichiometry and reaction equilibrium. 1-99 are reserved for user defined reactions. These reactions must have stoichiometric coefficients and reaction equilibrium constants entered through ChemTran.

**REACTION STOICHIOMETRY**  $i = (a_1*r_1 + a_2*r_2 + \dots = b_1*p_1 + b_2*p_2 + \dots)$

Enter reaction ID numbers. 100+ are reserved for library reactions. The user defined reaction is invoked in DESIGN II/ChemTran with the LIB REA = command

a<sub>1</sub>,a<sub>2</sub> are the stoichiometric coefficients for the reactants,  
r<sub>1</sub>,r<sub>2</sub> are the component ID numbers for the reactants,  
b<sub>1</sub>,b<sub>2</sub> are the stoichiometric coefficients for the products,  
p<sub>1</sub>,p<sub>2</sub> are the component ID numbers for the products,  
j is the reaction number.

**NOTE:** a<sub>1</sub>, a<sub>2</sub>,..., b<sub>1</sub>, b<sub>2</sub>,...,are all entered as positive values.

**EQUILIBRIUM CONSTANT** (units)  $i = TLL, TUL, A, B, C, D$

Enter coefficients for the equilibrium constant correlation for reaction  $i$  TLL and TUL are the lower and upper temperature limits of the range of validity of the correlation parameters.

A,B,C,D are the parameters in the correlation:

$$\ln(K) = A + B/T + C*T + D*\ln(T)$$

The units entered are for the temperature within the reaction equilibrium constant correlation must be either Rankine or Kelvin. The reaction equilibrium constant will also have composition units associated with it. These units MUST be molality.

**EDA**  $i,j = A_{ij}, A_{ji}, B_{ij}, B_{ji}, C_{ij}, C_{ji}$

Enter the interaction parameters for the Edwards model.

$$Beta(o)_{ij} = A_{ij} + B_{ij}*T + C_{ij}/T$$

where  $i$  and  $j$  are ion or molecule ID numbers.

**EDB**  $i,j = D_{ij}, D_{ji}$

Enter the interaction parameters for the Edwards model.

Presently, interaction parameters  $Beta(o)_{ij}$  and  $Beta(1)_{ij}$  parameters must be obtained from literature.

**HENRY'S CONSTANT** in **WATER** (options, units)  $i = TLL, TUL, \dots$

Enter coefficients in Henry's constant expression. Dimensions for the Henry's constant are pressure concentration. Again, liquid concentration MUST be molality.

Two of the following options are available for HEN WAT command.

**DATa**

Henry's constant for component  $i$  in water can be entered in "temperature-Henry's constant" pairs. The data will then be used to determine the regression constants for the Henry's constant. For this option temperature units should also be entered and they may be in C, F, R, or K. Using this option, the command takes the form:

**HEN WAT** (DAT,units) = TLL,TUL,H1,T1,H2,T2,....

**CONstants**

The regression coefficients for the Henry's constant can be entered directly. The correlation form is:

$$\ln(H) = A + B/T + C*T + D*\ln(T)$$

The temperature units should be Rankine or Kelvin. If this option is used the command takes the form:

**HEN WAT** (CON,units) = TLL,TUL,A,B,C,D

## ChemTran: Electrolyte Input File

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open... c:\designii\samples\chemtran\chemtr13.in to simulate this problem)**

```
AB123.
* DEFINE USER SPECIFIED REACTIONS
C- IDENTIFY LIBRARY AND ION COMPONENTS.
C-WATER, AMMONIA, HYDROGEN SULFIDE.
COMPONENT = 62, 63,50
C-      H+, OH-, HS-, NH4+,S=
ION COMPONENT = 9401, 9402, 9632, 9701,9631

C-CHOOSE THERMODYNAMIC METHOD.
EDWARDK
```

## Chapter 16

---

```
C- ENTER USER DEFINED LIBRARY REACTIONS.
LIBRARY REACTION = 101,104,105,109

C- DEFINE REACTION STOICHIOMETRY
C- REACTION 1 H2O <=> H+ +OH-
REACTION STOI 101=(1*62=1*9401+1*9402)
REACTION STOI 109=(1*63+1*62=1*9701+1*9402)
REACTION STOI 104=(1*50 = 1*9401 + 1*9632)
REACTION STOI 105=(1*9632 = 1*9401 + 1*9631)

C- ENTER EQUILIBRIUM CONSTANTS C1,C2,C3, and C4
EQU CON (R) 101=500,800,154.144,-24202.62,0.0,-22.4773,
EQU CON (R) 109=500,800,106.8259,-10645.3476,-0.006115561,-15.06399
EQU CON (R) 104=500,800,507.6058,-32462.496,0.0511013,-78.07186
EQU CON (R) 105=500,800,-234.4787,-730.8063,-0.03006157,33.88898

C- ENTER EDWARDS INTERACTION PARAMETERS FOR MOLECULE-MOLECULE PAIRS
EDA 63,63=-0.0260,-.0260,0.0,0.0,22.122,22.122
EDA 63,50=-0.1186,-0.1886,0.0,0.0,66.465,66.465
EDA 50,50=-0.2106,-0.2106,0.0,0.0,110.808,110.808

C- ENTER EDWARDS INTERACTION PARAMETERS FOR ION-ION PAIRS.
C- NOT NECESSARY FOR IONS OF SAME CHARGE.
EDA 9401,9402=0.208,0.208
EDA 9401,9632=0.194,0.194
EDA 9401,9631=.127,.127

EDA 9701,9402=0.060,0.060
EDA 9701,9632=0.046,0.046
EDA 9701,9631=-0.021,-0.021

EDB 9401,9402=0.65448,0.65448
EDB 9401,9632=0.61164,0.61164
EDB 9401,9631=0.40662,0.40662

EDB 9701,9402=0.20160,0.20160
EDB 9701,9632=0.15876,0.15876
EDB 9701,9631=-0.04626, -0.04626

C-ENTER EDWARDS INTERACTION PARAMETERS FOR ION-MOLECULE PAIRS.
EDA 63,9632=-0.06423,-0.06423,0.0001010,0.000101,0.0,0.0
EDA 63,9401=0.015,0.015,0.0,0.0,0.0,0.0
EDA 63,9402=-0.03801,-0.03801,0.0001169,0.0001169,0.0,0.0
EDA 50,9701=0.07932,0.07932,0.0000066,0.0000066,0.0,0.0
EDA 50,9401=0.017,0.017,0.0,0.0,0.0,0.0
EDA 50,9402=-0.05290,-0.05290,0.0001467,0.0001467,0.0,0.0
EDA 63,9631 = 0.032, 0.032,0.,0.,0.,0.

C- IDENTIFY CHEMICAL FILE NAME.
FILE NEW = AAAA,BBBB,CCCC
END
```

## ChemTran Correlating Mixture Data

### ChemTran: Introduction to Mixtures

---

Accurate process simulations for mixtures require a knowledge of the relationships among the variables temperature (T), pressure (P), vapor phase concentrations ( $Y_i; i=1,2,..N-1$ ), and liquid phase concentrations ( $X_i; i=1,2,..N-1$ ), where N is the number of components. This relationship is the basis for many process calculations; for example, K-value, bubble point, dew point, and flash calculations. For many chemical system predictive techniques based on theory and/or empirical correlations are not adequate to describe the interdependence of these variables. Simulations of these systems require correlations of experimental phase equilibrium data specific to the system.

ChemTran provides a fast and efficient way to obtain these correlations and apply the results in process calculations. There are several alternative input modes for transmitting V-L-E data to the program. These input modes may be used for mixtures consisting of two or more components. Once the data is encountered in an input file, it is reduced by a non-linear least squares procedure to a set of parameters and any other parameters applicable to the mixture are stored for future reference, as needed, when other mixture calculations are performed. In addition, by simply inserting a FILE NEW command in the input file (see *File Access Commands*) the user may instruct the program to store the results on a file for direct access by DESIGN II.

Default options in ChemTran will usually provide a converged set of correlation parameters for most binary mixtures and many ternary mixtures. More complex systems may necessitate some intervention on the part of the user in order to obtain an

accurate data fit. In order to permit this intervention, three different ways of altering the default options are provided in the form of simply coded user input statements.

This section offers a short presentation of V-L-E data correlation procedures covering the following topics:

1. Correlation equations
2. Data reduction procedures;
3. Data input modes, sources;
4. Examples.

Detailed descriptions of all the Input commands and correlation control commands mentioned for mixtures in this section are presented in *ChemTran: Mixture Command Details*. All of the pure component input statements described in *ChemTran Examples* and *ChemTran: Pure Component Property Generation* may be used in conjunction with the mixture data statements to place any necessary pure component data into the file.

---

## ChemTran: Correlation Equations , Procedures and Parameters

---

Although ChemTran is designed to greatly simplify the task of correlating V-L-E data, some knowledge of the basic principles is helpful. This will aid in understanding what types of mixture data are required for the optimization procedure, as well as provide insight into the methodology.

### ChemTran: V-L-E Equations

For systems at equilibrium, the connecting link between the variables T, P, (Y<sub>i</sub>), and (X<sub>i</sub>) are the relationships

$$Y_i P \phi_i^{\text{vap}}(X, Y, T, P) = X_i f_i^{\text{ss}}(T, P) \gamma_i(X, Y; \text{parameter})$$

for vapor – liquid equilibria, and

$$X_i^{(1)} \gamma_i^{(1)}(\text{liquid phase 1}) = X_i^{(2)} \gamma_i^{(2)}(\text{liquid phase 2})$$

for liquid – liquid equilibria, or in the case of equations of state

$$X_i \phi_i^{\text{liq}}(X, T, P; \text{parameters}) = Y_i \phi_i^{\text{vap}}(Y, T, P; \text{parameters})$$

X is the set of liquid phase concentrations (X<sub>1</sub>, X<sub>2</sub>... X<sub>N</sub>)

Y is the set of vapor phase concentrations (Y<sub>1</sub>, Y<sub>2</sub>... Y<sub>N</sub>)

N is the number of components in the mixture;

φ is the fugacity coefficient of i;

f<sub>i</sub><sup>ss</sup> is the standard state fugacity; and

γ<sub>i</sub> is the liquid phase activity coefficient of i.

These relationships form the ground work for the correlation of *ChemTran: V-L-E data systems*. The correlation procedure consists of evaluating the different functions and adjusting the parameters until the equations are satisfied (in at least squares sense) for every V-L-E data point. Evaluation of the functions has been discussed in *ChemTran: Selecting Correlations for Mixture Data*.

### ChemTran: Binary Parameters

The parameters which are adjusted to obtain the data fit are:

A<sub>ij</sub>, A<sub>ji</sub>, B<sub>ij</sub>, B<sub>ji</sub>, and C<sub>ji</sub>

There is one set of these parameters for each unique binary pair in a mixture. They alter the fundamental relationship given above by changing the concentration and temperature dependence of γ<sub>i</sub>. This dependence is expressed by the *ChemTran: RENon*, *ChemTran: UNIQUAC*, or *ChemTran: WILson* equations (only the first four parameters are used for WILson equations). Generally, only the A parameters are adjusted in the data reduction (the ChemTran default option); however, if there is a large temperature variation in the data, the B parameters may also be adjusted. This choice is left as a user option in ChemTran and is accomplished by inserting the appropriate FIX or VARY command in the input file.

Since the *ChemTran: RENon* and *ChemTran: WILson* equations have a theoretical basis, some physical meaning can be assigned to the parameters. This sometimes helps in forming judgments about the result of a data reduction calculation. The parameter A<sub>ij</sub> is very roughly a measure of the strength of the interaction between components i and j; the stronger the interaction the larger the value of A<sub>ij</sub>. If the system is close to ideal, then, in general, the absolute values of A<sub>ij</sub> will be small. For other systems the magnitude of A<sub>ij</sub> will depend on the nature of components i and j. Referring to *ChemTran: Regular Interactions* the absolute value of A<sub>ij</sub> would be largest for a mixture of components from GROUP IV.

RENOn's equations use the parameter C (the 'randomness' parameter) to adjust, in theory, for structure in liquids. As a very rough approximation, C is larger when the interactions are stronger. Thus, C would be expected to be larger for mixtures consisting of components from Group IV than for mixtures of components from Group I in *ChemTran: Regular Interactions* Table.

**NOTE:** For the PENg-Robinson, SOAVE and APISOAVE equations, there will be one A and one B parameter. The B<sub>ij</sub>

parameter describes the temperature dependency.

### **ChemTran: Equilibrium Input Commands, Sources, and Requirements**

Several forms of phase equilibrium data may be entered into ChemTran for data reduction. In general, these forms comprise two types:

1. T versus P versus Y (vapor concentration) versus X (liquid phase concentration) and
2. T versus P versus X.

In both cases T or P may be constant for a set of data while the other variables vary.

All of the different combinations of variables which may be entered in an input file and the corresponding input command (see *ChemTran: Mixture Command Details* for input command syntax) are summarized below.

#### **ChemTran: T-P-Y-X, T-Y-X, P-Y-X Data Commands**

These input commands are used to enter V-L-E data where both the vapor and liquid phase concentrations are known. The T-Y-X command is used for data taken at constant pressure and the P-Y-X command for data taken at constant temperature. When both T and P vary, the T-P-Y-X command is used.

#### **ChemTran: T-P-Y-X-X, T-Y-X-X, P-Y-X-Y Data Commands**

These input commands are used to enter vapor-liquid-liquid-equilibrium data. They must be used with either the RENon or UNIQUAC option. The T-Y-X-X command is used for constant pressure data and the P-Y-X-X command for constant temperature data. When both T and P are varying the T-P-Y-X-X command can be used.

#### **ChemTran: T-P-X, T-X, P-X Data Commands**

For some experimental configurations only T, P and liquid phase concentrations are measured even when the system consists of vapor and liquid in equilibrium. This type of data is usually referred to as solubility data and is entered with the T-P-X, T-X, or P-X input commands. Data collected at constant pressure are entered on a T-X command and data collected at constant temperature on a P-X command. If both T and P are permitted to vary, then the data is entered on a T-P-X command. These commands **cannot** be used when the data represents liquid phases only - a vapor phase must be present. The vapor phase concentrations will be accounted for by algorithms contained in ChemTran.

#### **ChemTran: T-X-X, T-X-X-X Data Commands**

##### **T-X-X Data**

Data for partially miscible liquid-liquid systems may be entered with this command. For these systems the temperature and concentrations of both liquid phases must be entered. Only the RENon and UNIQUAC correlation equations may be used for the reduction since WILson's equations do not account for immiscibility.

##### **T-X-X-X Data**

This command can be used to enter mixture data on systems with three liquid phases in equilibrium. Only the RENon and UNIQUAC option can be used for the data regression. The temperature and compositions for all three liquid phases must be entered.

#### **ChemTran: Data Base Sources for VLE and LLE Data**

Experimental VLE and LLE data can be obtained from WinSim's (via internet: support@winsim.com) interactive database system MixMaster (not marketed as a product). This database contains two extensive and complete collections of data until 1985:

1. The Dortmund Data Bank collected by J. Gmehling and U. Onken at the University of Dortmund in Dortmund, Germany.
2. The Lyngby Data Bank collected by A. Fredenslund and co-workers at the Denmark's Tekniske Hojskole in Lyngby, Denmark.

Additionally,

The DETHERM Internet client gives access to thermophysical property data included in the DETHERM online database maintained by DECHEMA e.V., Frankfurt am Main, Germany. For further information look at DECHEMA's website on <http://www.dechema.de>.

The Dortmund Data Bank [www.ddbst.de](http://www.ddbst.de) contains virtually all VLE data reported in the literature starting in the 1890's for chemicals boiling above 0 degrees C. Similarly, the Lyngby Data Bank contains virtually all the LLE and LLE data reported in the literature.

Together, these Data Banks have the largest numerical databases for thermophysical property data with 2.85 million data sets for around 100,000 systems (about 16,000 pure substances and 84,000 mixtures) contains phase equilibrium data, electrolyte data, pure substance and mixture properties. This is now exclusively offered by DECHEMA for a fee per data download (data searches are free) at [www.dechema.de](http://www.dechema.de). We highly recommend you to use this comprehensive resource for all current and old component mixture (solubility, VLE, LLE, and other physico-chemical data) information.

#### **ChemTran: Data Requirements**

Regardless of the type of V-L-E data entered in an input file there are two requirements which it should satisfy:

1. There should be sufficient data to permit determination of all parameters which are adjusted; and

- The data should, as closely as possible, span the ranges of temperature, pressure and concentrations of the process simulation in which the correlation is used.

ChemTran provides a check for requirement (1) and will print a message when it is not satisfied. Careful thought and preparation on the part of the user are necessary to satisfy the second requirement. The minimum number of data points which are required for successful correlation varies with the type of data and the number of adjustable parameters.

**ChemTran: Table 6.1. Minimum Number of Parameters Permitted for Reducing V-L-E Data** summarizes the conditions which must be met. For a ternary mixture, there are 3 binary interactions. If there are two adjustable parameters per binary then a total of six parameters will be varied to fit the data. The relationship in **ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data**, indicates a minimum of two T-P-Y-X data points would be required or, if T-P-X data is used, a minimum of six data points.

**ChemTran: Table 6.1. Minimum Number of Parameters Permitted for Reducing V-L-E Data**

<u>Data</u>	<u>Type Condition</u>
T-P-Y-X, P-Y-X, and T-Y-X	(No. of components) * (No. of Data points) $\geq$ No. of parameters
T-P-X, T-X, and P-X	No. of data points $\geq$ No. of parameters
T-X-X	(No. of components) * ((No. of Data points $\geq$ No. of parameters
T-P-Y-X-X, T-Y-X-X, P-Y-X-X, and T-X-X-X	(No. of components) * (No. of Data points) $\geq$ No. of parameters

Only the theoretical minimum data point requirements are met by the conditions presented in **ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data**. More data points are required to insure a faithful representation of the vapor-liquid equilibrium in a mixture for all possible values of T,P,X, and Y. The correlation should not be extrapolated far beyond the temperature range of the data. Pressure extrapolations can be handled much better, but the best results will be obtained when the pressure range spanned by the data is close to that of the simulation. In general, concentrations should cover the range of the simulation. However, particular care must be taken to enter sufficient data to represent regions where the relative volatility approaches unity. The accuracy of the fit in these regions of concentration has a strong effect on the number of trays needed in the simulation of a distillation column.

### **ChemTran: Reduction of Data**

For most cases, ChemTran reduces the task of correlating mixture data to inserting one to three types of input statements into the input file. (details for entering data with these commands are presented in **ChemTran: Correlating Mixture Data**.)

- An input command for the data (T-P-Y-X, T-Y-X, T-X, etc.);
- A command to specify the K-value option: WILson, PENg-Robinson, UNIQUAC, RENon, APISOAVEK or SOAVEK.
- An OBJective FUNction command to indicate which function of the input variables is to be used for the non-linear least squares minimization.

If the mixture consists of components which are not in the **Database Components**, then it will be necessary to enter the appropriate pure component commands discussed in **ChemTran: Pure Component Command Details** and **ChemTran: Pure Component Property Generation**. These commands may also be used to override data for components in the Data Base if the user desires.

Data correlation for some mixtures, particularly those with more than two or three components, may require additional steps to obtain a set of converged correlation parameters. These consist of:

- Altering the default options for setting initial values of parameters with the RENon, WILson, PENg, UNIQUAC, APISOAVE, SOAVE, or BINary command;
- Altering the default options, using a FIX or VARY command, for selecting parameters which are to vary in the minimization procedure.

The syntax for these commands is presented in **ChemTran: Mixture Command Details**.

These five steps are all that is required for the correlation of mixture data using ChemTran. Each step is associated with a type of input command or correlation control command and is executed by entering that command with the appropriate data into an input file. Thus, a series of one (1) to five (5) statements in the input file accomplishes the data reduction.

### **ChemTran: Comparison of WILson and RENon Equations**

There are few rigid criteria for choosing between the WILson or RENon equations for correlation of data. The functional forms, presented in **ChemTran: Selecting Correlations for Mixture Data**, are similar with the exception that the WILson equations employ the pure component liquid volumes in their formulation. WILson's equations have some advantage over those of RENon because there are fewer parameters to adjust; two (2) to four (4) compared to two (2) to five (5) for RENon's equations. However, only RENon's equations are applicable to systems of limited miscibility and must be used with liquid-liquid data (T-X-X). WILson's equations are generally recommended for alcohol-hydrocarbon systems if phase splitting does not occur.

Comparisons of the WILson and RENon equations for several mixtures reveal no clear trend in the types of chemical systems where one might be preferable to the other.

## ChemTran: Objective Functions for V-L-E Data

Parameter optimization is accomplished by locating the minimum of a function, formed from the input variables T,P,X and Y and the relationship presented in *ChemTran: Binary Interaction Coefficients Table*. This function may be formed in several ways and these are summarized in *ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data*. The type of objective function used for the data reduction is a user option which is entered on the OBJective FUNction command. As is shown in the table, for some forms of input data the choice of objective function is restricted.

The functions listed in *ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data* are formed by summing the squares of the deviations of the estimated property (those listed in the first column of the table) from the value obtained from the data. Thus, when the total pressure is chosen as the objective function, errors in pressures calculated from the correlation are minimized; when K-values are chosen, the errors in estimated K-values are minimized. Since some properties may be more important than other for a given application, it may be desirable to choose the objective function based on the property that is most important to the process simulation in which the correlation will be used. In ChemTran the default option for the objective function is 3, for K-values, with the exceptions noted in *ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data*. If you do not specify an objective function, ChemTran will choose option 3 or 1, whichever is appropriate, for each data set which is to be fitted.

**ChemTran: Table 6.2. Objective Functions for Reduction of V-L-E Data**

Function	Code	Functional Form
total <sup>2</sup> pressure	1	$\sum_{i=1} \{(P - P_i)\}^2$
relative volatility	2	$\sum_{i=1} \sum_{j=1} \left\{1 - \frac{(\alpha_{1ij})_{\text{calc}}}{(\alpha_{1ij})_{\text{exp}}}\right\}^2$
K-Values <sup>3</sup>	3	$\sum_{i=2} \sum_{j=1} \left\{1 - \frac{(K_{ij})_{\text{calc}}}{(K_{ij})_{\text{exp}}}\right\}^2$
K-values and relative volatility <sup>3</sup>	4	$\sum_{i=1} \left[ \left\{1 - \frac{(K_{ij})_{\text{calc}}}{(K_{ij})_{\text{exp}}}\right\}^2 + \sum_{j=2} \left\{1 - \frac{(\alpha_{1ij})_{\text{calc}}}{(\alpha_{1ij})_{\text{exp}}}\right\}^2 \right]$
activity coefficient <sup>2</sup>	5	$\sum_{i=1} \sum_{j=1} \left\{1 - \frac{(\gamma_{ij})_{\text{calc}}}{(\gamma_{ij})_{\text{exp}}}\right\}^2$
K-Values weighted by $Y_i^3$	6	$\sum_{i=1} \sum_{j=1} \left\{1 - \frac{(K_{ij})_{\text{calc}}}{(K_{ij})_{\text{exp}}}\right\}^2 Y_{ij}$
Fugacity divided by pressure <sup>4</sup>	7	$\sum_{i=1} \sum_{j=1} \{X_{ij} \phi_{ij}^{\text{liq}} - Y_{ij} \phi_{ij}^{\text{vap}}\}$

<sup>1</sup> summations are over components and data points.

<sup>2</sup> may not be used with equations of state (such as Peng-Robinson, APISOAVE, or SOAVE).

<sup>3</sup> may not be used with T-P-X, T-X or P-X data.

<sup>4</sup> may not be used with activity coefficient correlations (such as WILson, RENon, or UNIQUAC).

**NOTE:** ChemTran has an internal objective function for Liquid-Liquid data reduction.

## ChemTran: Changing Parameter Default Options

The optimization procedure for the objective function requires the specification of a set of parameters which are to be varied for each binary interaction, and initial values for each of the parameters. Parameters which are not allowed to vary, but are still involved in the correlation must also be set to a specific value. ChemTran contains defaults for selection of the variable parameters and the initial values of all parameters. These default conditions are sufficient for the correlation of data for most binary mixtures and many ternary mixtures. They are summarized in *ChemTran: Table 6.3. Default Conditions for V-L-E Optimization Parameters*. As the table indicates, all A and B parameters are set to zero initially. The RENon 'randomness' parameters are set to 0.2 initially. Usually the A parameters for each binary interaction in the mixture are the ones allowed to



vary. This is usually all that is necessary for minimizing the objective function formed from binary data when the temperature range of the data is small. If the temperature range is large, the B parameter may be allowed to vary as a user option.

**ChemTran: Table 6.3. Default Conditions for V-L-E Optimization Parameters**

Parameter	Initial Value	Varied	Comments
A <sub>ij</sub>	0.0	Yes	- - -
A <sub>ji</sub>	0.0	Yes	- - -
B <sub>ij</sub>	0.0	No	the B's are used when
B <sub>ji</sub>	0.0	No	the data spans a large temperature range
C <sub>ij</sub> *	0.2	No	for RENon equation only
C <sub>ji</sub> *	0.2	No	for RENon equation only

\*where the C parameters are subject to the condition  $C_{ij} = C_{ji}$

**NOTE:** The PENg-Robinson, SOAVEK, and APISOAVEK equations only have one A and B parameter.

### ChemTran: Initial Values of Parameters

ChemTran performs the V-L-E data reduction by searching for values of the variable parameters which minimize the objective function. This search works best when the initial values of the parameters are close to their value at a minimum of the function. Normally, for binary data the default initial settings are sufficient to obtain a set of converged parameters. For mixtures with more than two components, it is desirable to enter initial guesses with the appropriate RENon, PENg, WILson, UNIQUAC, APISOAVE or SOAVE command, depending upon the equation option chosen, for as many binary interactions as possible. This requires first fitting binary data, then using the resulting parameters to fit the mixture data. When this is done, all options and pure component data used in the binary data reduction should be the same for the ternary analysis.

### ChemTran: Changing the Variable Parameters

In some cases, the reduction of mixture data may require a different set of variable parameters than is specified by the default options of ChemTran. These default options may be changed when using a FIX and/or a VARY command. One such case occurs when there is a large amount of data spanning a large temperature range. Then the VARY command may be used to allow the B parameters to vary as well as the A parameters. In addition, the RENon equations may not provide as good a fit as the WILson equations for some types of mixtures unless the C parameters are permitted to vary. In using these commands, it should be kept in mind that the fewer parameters that are permitted to vary, the faster the search procedure will proceed. If there is some difficulty in obtaining a set of converged parameters for a set of data it is possible to allow some parameters to vary until a relative minimum is found, then fix these and let others vary until a better minimum is found. This procedure may be applied to mixtures where parameters for some binary interactions are known while other are not. This data would be correlated by fixing the known parameters, then letting the unknown parameters vary. In some cases, further reduction in the error may be obtained by then letting all the parameters vary.

*Example 1.* Correlate ternary data using ChemTran for the system carbon tetrachloride, benzene, and isopropyl alcohol.

These are components contained in the *Database Components*, and do not require the entry of any pure component data.

The input file consists of the following commands:

```
AB123.
*FIT V-L-E DATA CCL4 + BENZENE + ISOPROPYL ALCOHOL
COM = 1027, 40, 1019,
WILSON
WIL 1027, 40 = 161, 200, 00, 0, 0
WIL 1027, 1019 = 161, 110, 1200, 0, 0
WIL 40, 1019 = 61, 844.633, 1163.676, 0, 0
T-P-Y-X (MMH,C) 1027, 40, 1019 =
73.50, 760.0, .0540, .4700, .0320, .3630,
71.90, 760.0, .0480, .5120, .0340, .4560,
72.00, 760.0, .1000, .4720, .0710, .4300,
70.20, 760.0, .5080, .0660, .710, .0520,
71.20, 760.0, .4710, .0710, .3010, .0540,
71.30, 760.0, .420, .110, .3130, .0830,
73.80, 760.0, .4160, .4370, .4290, .5280,
75.10, 760.0, .4580, .4490, .4680, .060,
75.50, 760.0, .4200, .4870, .420, .5550,
75.90, 760.0, .1000, .7840, .0920, .8680,
72.80, 760.0, .0960, .6270, .0920, .8680,
71.60, 760.0, .0880, .5630, .0780, .6210,
FIL NEW = CCL4C6H6.DATA
END
```

The Input commands in the preceding example serve the following purposes:

1. The first command is the Account number.
2. The second command is a title which will appear at the top of every output page.
3. The third command lists the component ID numbers.
4. The fourth command indicates that the WILson equation is to be used to correlate the data.

## Chapter 16

- The next three commands furnish optional initial values for the A and B parameters.
- The next 13 commands provide the V-L-E data and indicate the temperature, pressure, vapor phase mole fractions, liquid phase mole fractions which are varying; also the units are degrees C and mm of Hg. Temperatures are listed in the first column and pressures in the second column. Vapor phase concentrations of components CCl<sub>4</sub> and benzene are listed in columns 3 and 4. Similarly, liquid phase concentrations are listed in columns 5 and 6. It is important to note that the spacings shown here are merely for convenience and not required; other than the four blanks at the beginning of each continuation line.
- A FIL NEW command is entered to store results for access by the DESIGN II program.
- The last command is an END which must be the last statement of an input file.

### ChemTran: Mixture Command Details

#### ChemTran: Activity Coefficients at Infinite Dilution

**ACT**ivity (units,options) i,j=data list

This command is used to convert infinite dilution activity coefficients to WILson, RENon, or UNIQUAC binary interaction parameters. The options are as follows:

<u>Options</u>	<u>Data List</u>	<u>Data List</u>
DATA		T, $\gamma_i^\infty$ , $\gamma_j^\infty$
UNIFAC		T
LLU		T

If the DATA (default option is used then infinite dilution activity coefficients must be entered at a temperature T. When the UNIFAC option is used infinite dilution activity coefficients are generated by the UNIFAC correlation at temperature T. When the LLU option is specified, UNIFAC is used to calculate the infinite dilution activity coefficients, however, a liquid-liquid equilibrium data bank is used. Magnussen, T., Rasmussen, P., and Fredenslung, A., 'UNIFAC Parameter Tables for Prediction of Liquid-Liquid Equilibria', Industrial Engineering and Chemical Process Design and Development, Vol. 20, 1981.

*Example 1.* **ACT** 200, 205 - 30., 2.71, 3.26,

In this example the following data are entered:

$$\lim_{X_{200} \rightarrow 0} \gamma_{200} = \gamma_{200}^\infty = 2.71$$

$$X_{200} \rightarrow 0$$

$$\lim_{X_{205} \rightarrow 0} \gamma_{205} = \gamma_{205}^\infty = 3.26$$

$$X_{205} \rightarrow 0$$

$$\text{Temperature } T = 30^\circ\text{F}$$

where 200 and 205 are the user assigned component ID numbers for this binary pair.

*Example 2.* **ACT** (C,UNIFAC) 7033, 1021 = 125,

This command will produce UNIFAC estimates of binary interaction parameters at 125 °C.

**NOTE:** See *ChemTran: Unified Group Contribution Technique* for commands for entering the UNIFAC group structures for non-standard components.

#### ChemTran: Excess Enthalpy Commands

**HE - T - X** (units) i, j = HE<sub>1</sub>, T<sub>1</sub>, X<sub>11</sub>, HE<sub>2</sub>, T<sub>2</sub>, X<sub>21</sub>, ...

Excess enthalpy or heat of mixing data are entered with this command. HE is the value of the excess enthalpy at temperature T and mole fraction X of the component i, where i is the component ID number.

**Note:** When excess enthalpy data is entered with the HE-T-X command, please also use **EXC LAT** command. More details are at [ChemTran: Enthalpy Data Systems](#) and [ChemTran: Excess Enthalpy Data](#).

*Example 1.* Enter the following excess enthalpy data for HCl and H<sub>2</sub>O.

<u>(BTU/LBMOL)</u>	<u>T°R</u>	<u>mol fraction of HCl</u>
-5528.1	509.67	.184
-7719.3	509.67	.263
-12383.0	509.67	.464
-5662.	545.66	.184
-9813.0	545.55	.336

**HE-T-X**(BTU/LBMOL,R) 1017,62=-5528.1, 509.67, .184,  
-7719.3, 509.67, .263,  
-12383, 509.67, .464,

-5662.2, 545.66, .184,  
-9813, 545.66, .336

### **ChemTran: FIX Binary Interaction Parameters**

**FIX** i, j = data list

This command is used in conjunction with the *ChemTran: VARY Binary Interaction Parameters* command to alter the default options in ChemTran that are used to select adjustable parameters in fitting V-L-E data. The defaults are:

A<sub>ij</sub> and A<sub>ji</sub> vary  
B<sub>ij</sub> and B<sub>ji</sub> are fixed  
C<sub>ij</sub> and C<sub>ji</sub> are fixed (C<sub>ij</sub> = C<sub>ji</sub> for Renon equations).

Parameters may be fixed by entering their symbols in the data list portion of the FIX command.

*Example 1.* Let A<sub>ij</sub> be the only adjustable parameter for a V-L-E Data reduction for components 200 and 210.  
**FIX** 200, 210 = A21

*Example 2.* Fix the parameters A<sub>ij</sub> and A<sub>ji</sub>, vary B<sub>ij</sub> and B<sub>ji</sub> for components 205 and 207.  
**FIX** 205, 207 = A12, A21  
**VARY** 205, 207 = B12, B21

### **ChemTran: VARY Binary Interaction Parameters**

**VARY** i, j = data list

This command is used in conjunction with the *ChemTran: FIX Binary Interaction Parameters* command to alter the default options in ChemTran that are used to select adjustable parameters in fitting VLE data.

The defaults are:

A<sub>ij</sub> and A<sub>ji</sub> vary  
B<sub>ij</sub> and B<sub>ji</sub> are fixed  
C<sub>ij</sub> and C<sub>ji</sub> are fixed (C<sub>ij</sub>=C<sub>ji</sub> for Renon equations).

Parameters may be allowed to vary by entering their symbols in the data list portion of the VARY command.

*Example 1.* For Components 200 and 205 vary the B<sub>ij</sub> and B<sub>ji</sub> parameters.  
**VARY** 200,205 = B12,B21

*Example 2.* For components 200 and 205 vary B<sub>ij</sub> and B<sub>ji</sub> parameters. Fix the parameters A<sub>ij</sub> and A<sub>ji</sub>.  
**VARY** 200,205 = B12, B21  
**FIX** 200,205 = A12,A21

### **ChemTran: GRaph Commands**

**GR**aph variable 1 - variable 2 (options,units) i, j = data

This command may be used to generate plots on a line printer for binary VLE data. Presently, variable 1 is restricted to Y (vapor phase mole fraction of component 1), P (pressure for dew and bubble points), T (temperature for dew and bubble points), or Act (liquid phase activity coefficient). The ordinate, variable 2, is restricted to X (Liquid phase mole fraction of component i).

This Permits four types of graphs:

<b>Command</b>	<b>Function</b>
GRaph Y-X	Y vs. X at constant T or P
GRaph T-X	T vs. X at constant P
GRaph P-X	P vs. X at constant T
GRaph A-X	$\gamma$ vs. X at constant T or P

The full slate of units for temperature and pressure (see *Input Units: Options*) are available with these commands. Other options are:

<b>Options</b>	<b>Function</b>
PREssure	graphs are to be made at constant pressure; the pressures are placed in the data list
TEMperature+	graphs are to be made at constant temperature; the temperatures are placed in the data list
YES	appropriate experimental data points are placed on the graph (indicated by the letter E)
NO Data+	no experimental points should be placed on the graph
WIDe	plot graph with width of 120 characters
NARrow+	plot graph with width of 72 characters

**NOTE:** Default options do not have to be entered and are marked with a '+' sign superscript.

The TEM and PRE options are only necessary with Y-X and A-X plots. Since these plots are either isotherms or isobars the

## Chapter 16

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temperature or pressure must be entered in the data list. Multiple plots, at several temperatures or pressures, can be made with one graph command by entering the desired temperatures or pressures in the data list.

*Example 1.* Generate three vapor composition vs. liquid composition graphs for ethanol and water at 760, 800, and 900 mmHG.

**GRA Y-X** (NOD, MMHG, PRE) 1012,62 = 760,800,900

In this example no experimental data points will be plotted on the graph and it will be 72 characters wide.

*Example 2.* Generate a P versus X plot for isopropanol-methanol at 66, 69, 72, and 75 degrees C.

**GRA P-X** (YES,C,WID) 1019,1021=66,69,72,75

In this example experimental data will be plotted on the graph and it will be 120 characters wide.

### ChemTran: IDEal Mixture Commands

#### IDEal Binary Interactions

**IDEal** (units) i,j

Entry of this command into the input file causes the interactions between components i and j to be treated as ideal. That is the interaction parameters are set to zero. This is an automatic procedure in ChemTran if no other specification of the interaction between i and j has been made.

#### IDEal VAPor Specification

**IDEal VAPor**

This command instructs ChemTran to treat the vapor phase as ideal (fugacity coefficients are set equal to one) in all multi-component data processing. It is a reasonable option to use at low pressures and reduces computation time by about 30%.

### ChemTran: K-Value Options

Enter the K-value correlation you wish to use for data regression or equilibria prediction.

**APISOAVE K**

**PENg K**

**RENon**

**SOAVE K**

**UNIFAC K** (not used for data regression)

**UNIQUAC K**

**WILson**

### ChemTran: APISOAVE Parameters

**APISOAVE** (units) i,j = A<sub>ij</sub>, B<sub>ij</sub>

This command is used for entering APISOAVE parameters to describe the binary interaction between components i and j. If no other data are entered (binary, ternary, etc.) then these constants will be used to describe the i-j interaction. This command may be used to add to or override the binary interaction parameters built into the APISOAVE correlation.

The B<sub>ij</sub> parameter describes the temperature dependency of the data fit.

*Example 1.* Enter interaction parameters for CO<sub>2</sub> and methanol for the APISOAVE equation. The value from the literature is .017.

**APISOAVE** 49,1021=0.017

### ChemTran: Hildebrand Interaction Parameters

**SCA**tchard Hildebrand

Enter this command to have interaction constants for WILson, RENon, or UNIQUACK estimated from regular solution theory for all binary pairs for which no VLE data was entered. The interaction constants determined in this manner are labeled with \*REG on the printed output.

### ChemTran: MODified PENg K Method

**MODified PENg K** (option)

This command specifies the modified Peng-Robinson thermodynamic correlation that is applicable for high pressure non-ideal systems. See *ChemTran: Modified Peng Robinson Equation of State* for a description of this method.

**Options**

**Mixing Rule**

Standard

Standard Mixing Rule

MAR

Margules non-symmetric mixing rule

When specifying this method, it is essential that kappa parameters be specified. Kappa parameters are specified with the KMODPEN command. See *ChemTran: Kappa Parameter* for instructions on using this command. If kappa parameters are not specified with the KMODPEN command the method will default to the standard Peng-Robinson equation of state.

**MOD PEN**  $i, j = A_{ij}, A_{ji}, B_{ij}, B_{ji}$ 

Enter interaction parameters for the modified Peng-Robinson equation which have been regressed in earlier ChemTran runs or which are starting estimates of the values to be regressed.

**ChemTran: PENg Robinson Parameters****PEN**  $i, j = A_{ij}, B_{ij}$ 

This command is used to enter interaction coefficients for the Peng-Robinson equation.

*Example 1* Enter the Peng-Robinson interaction parameter for carbon dioxide and iso-butane. The value from the literature is .130.

**PEN** 49, 5 = .130

**ChemTran: RENon Parameters****RENon** (units) $i, j = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}, C_{ij},$ 

This command is used to enter RENon binary interaction parameters for the pair of components  $i$  and  $j$ . The average temperature for the variables is  $T$ . If no other data are entered (binary, ternary, or other, VLE data) then these parameters will be used to describe the interactions. Otherwise, they will be used as first guesses in regressing VLE data to RENon's equations. The equations are presented and discussed in detail in *ChemTran: Renon Equations*. As a reminder, the variables serve the following purpose:

1.  $A_{ij}$  and  $A_{ji}$  are the parameters for the short form of RENon's equations.
2.  $B_{ij}$  and  $B_{ji}$  are the parameters for the extended form and are usually held constant, unless there is a large temperature variation.
3.  $C_{ij}$  and  $C_{ji}$  scale the A's and B's.

The default initial values in ChemTran are:

$A_{ij} = 0;$        $B_{ij} = 0;$        $C_{ij} = 0.2;$

$A_{ji} = 0;$        $B_{ji} = 0;$        $C_{ji} = 0.2;$

$B_{ij}, B_{ji}, C_{ij}$  and  $C_{ji}$  are held fixed with the condition that  $C_{ij} = C_{ji}$

*Example 1.* **REN** (CAL/GMOL,C) 205,210=50.,-133.,976,2\*0,0.2,

In this example the data entered is:

$$\begin{aligned} A_{205,210} &= -133. \\ A_{210,205} &= 976. \\ B_{205,210} &= B_{210,205} = 0. \\ C_{205,210} &= C_{210,205} = 0.2 \end{aligned}$$

at an average temperature of 50.0 °C

**ChemTran: UNIFAC K Parameters**

Specifies the UNIFAC group contribution method used to predict non-ideal vapor liquid equilibria. This command is not used when regressing equilibria data rather it is used only if the user wants to plot VLE data with the GRaph Y-X,..etc. commands or to predict VLE data with the T-X,..etc. commands. Since the structure of all ChemShare library components is stored in the component database, ChemTran will automatically determine which UNIFAC groups are present for all components in the components list. The UNIFAC method is not applicable to all components and if there is a component specified that has a non UNIFAC group, ChemTran will provide an error message stating which component is not represented in the UNIFAC method.

**UNIFAC K Available Options**

The user may select one of two UNIFAC data banks by including one of the following commands:

**VLE UNIFAC = 1**

**VLE UNIFAC = 2** (default)

The first option specifies a data bank that includes the 1983 revision of the UNIFAC groups (Macedo, E.A., Weidlich, V., Gmehling, J., and Ramsmussen, P., 'Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension 3', Industrial Engineering and Chemical Process Design and Development, Vol. 22, 1983. Although this is older and less accurate data, ChemShare has maintained this for those customers who need to maintain continuity of results.

The second option specifies a data bank that includes the 1987 revision of the UNIFAC groups (Rasmussen, P., Tiegs, D., Fredenslund, A., and Gmehling, J.), 'Vapor-Liquid Equilibria by UNIFAC Group Contribution. Revision and Extension 4', Industrial Engineering and Chemical Process Design and Development, Vol. 26, 198.

See *ChemTran: UNIFAC Estimation Technique for Activity Coefficients* for listing of all available UNIFAC groups.

**ChemTran: UNIQUAC K Parameters**

## Chapter 16

UNIQUAC (units) $i, j, k, \dots = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}$

This command is used to enter interaction parameters for the binary pair  $i$  and  $j$ .  $T$  is the average temperature of the system. The  $B_{ij}$  parameters are used for temperature dependence. *ChemTran: UNIQUAC Equations* illustrate the correlations used.

*Example 1.* Enter the UNIQUAC parameters for methanol and water. The parameters from the literature are

$$\begin{aligned}A_{ij} &= -243.3736 \text{ CAL/GMOL} \\A_{ji} &= 346.5601 \text{ CAL/GMOL}\end{aligned}$$

and the average temperature is  $39.9^\circ \text{C}$

**UNIQUAC (CAL/GMOL,C)** 1021,62=39.9,-243.3736,346.5601

### UNIQUAC Size Parameters

**R UNIQUAC**  $i =$

**Q UNIQUAC**  $i =$

Use these commands to enter the molecular volume parameter ( $r$ ) and area parameter ( $q$ ) for component  $i$  for use in the UNIQUAC equation. This information is automatically supplied for Data Base components and for non-standard components. These values will also be calculated from the STRUcture input, where appropriate. The  $R$  and  $Q$  parameters are related to the Van de Waal group volume ( $V_i$ ) and group surface area ( $A_i$ ) by the expressions:

$$\begin{aligned}R_i &= V_i/15.17 \\Q_j &= A_j/(2.5 \times 10^9)\end{aligned}$$

where

$$V_i \text{ is in cm}^3/\text{gmol} \text{ and } A_i \text{ is in cm}^2/\text{gmol}.$$

If no parameters are entered for non-condensables, they will be assigned a value of zero for  $R$  and  $Q$ . This works well for hydrogen, nitrogen, oxygen, carbon monoxide, argon and methane. For hydrogen sulfide and ammonia,  $R=1$  and  $Q=1$  have been used with some success.

**NOTE:** Values entered for any component should be generated in strict accordance with the UNIQUAC method. See the following reference for details:

Fredenslund, A., Gmehling, J., and Rasmussen, P., Vapor-Liquid Equilibria Using UNIFAC, A Group Contribution Method, Elsevier Scientific Publishing Co., New York, 1977.

### ChemTran: VAN Laar Parameters

**VAN** (units) $i, j = T, A_{ij}, A_{ji}$

Van Laar parameters are entered on this command to describe the interaction between components  $i$  and  $j$ . ChemTran converts these parameters to the equivalent WILson, or RENon or UNIQUAC parameters. The average temperature of the interaction is  $T$ . Van Laar constants are described by the following *ChemTran: VanLaar Equations*:

$$\log \gamma_i = A_{ij} X_j^2 / (A_{ij} X_i / A_{ji} + X_j)^2$$

$$\log \gamma_j = A_{ji} X_i^2 / (A_{ji} X_j / A_{ij} + X_i)^2$$

where  $\gamma$  is the activity coefficient.

*Example 1.* **VAN (C)** 205,209 = 25., .2039, .1563,

For this example:

$$A_{205}, A_{209} = .2039$$

$$A_{209}, A_{205} = .1563$$

$$T = 25.0^\circ \text{C}$$

### ChemTran: WILson Parameters

**WILson** (units) $i, j = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}$

This command is used for entering WILson parameters to describe the binary interaction between components  $i$  and  $j$  at an average temperature of  $T$ . If no other data are entered (binary, ternary, etc.) then these parameters will be used to describe the  $i$ - $j$  interaction. Otherwise, they will be used as initial guesses for data reduction to WILson equations. As a summary

1. the  $A$ 's are for the short form of WILson's equations;
2. the  $B$ 's are for the extended WILson equations and are used only if there is data for a wide range of temperatures.

Please see *ChemTran: Wilson Equations* and the significance of the constants for a more complete discussion of these parameters.

The default conditions for variation of these parameters and their initial values for data reduction are

$A_{ij} = 0; B_{ij} = 0;$   
 $A_{ji} = 0; B_{ji} = 0;$   
 $A_{ij}$  and  $A_{ji}$  varied;  
 $B_{ij}$  and  $B_{ji}$  fixed.

*Example 1.* Enter WILson parameters for methanol (1021) and water (62). The values from the literature are 126.3014 calories per gram-mole for methanol-water and 289.3537 calories per gram-mole for water-methanol at an average temperature of 36.4 C.

WIL(CAL/GMOL,C) 1021,62-36.4,126.3014,289.3537

### **ChemTran: OBJective FUNction Command**

**OBJective FUNction** = key

This command tells ChemTran what function to minimize in any multi-component vapor-liquid-equilibrium data correlation. The options are:

<u>KEY</u>	<u>Objective function Description</u>
1*	sum of the squares of pressure deviations
2*	sum of the squares of relative volatility deviations
3	sum of the squares of K-value deviations
4*	sum of the squares of K-value deviation for first component and relative volatility deviations for remaining components
5*	sum of the squares of activity coefficient deviations
6	same as 3, but weighted by the vapor mole fraction
7+	sum of squares of difference of fugacity in vapor and liquid phase

\* keys 1, 2, 4, 5 are used only with WILson, RENon, or UNIQUAC equations.

+ used with PENG-ROBINSON, APISOAVE, and SOAVE equations

All deviations are relative differences between calculated and experimental values.

Options 2, 3, 4, 5, and 6 can be used only with T-P-Y-X, T-Y-X (pressure constant), or P-Y-X (temperature constant) type data. All multi-component data will be processed with the same objective function for a single case. ChemTran **defaults** to key=3.

*Example 1.* In this example, ChemTran is being instructed to minimize the sum of deviations of activity coefficients.

**OBJ FUN** = 5,

### **ChemTran: TABLE Options**

**TABLE VARIABLE** (OPTIONS, UNITS) i,j,k,..

This command is used to control output of tables showing comparisons of various calculated and experimental variables associated with VLE data reduction. If no command is entered this output is automatically printed.

Both bubble point temperature and pressure are calculated and compared with the experimental data points. For each of these calculations the resulting vapor phase composition, K-values, and activity coefficients are also compared with experimental data. In addition, a table is printed listing the standard state fugacity, vapor phase fugacity coefficient, and liquid phase activity coefficient for each component and data point.

All table printout can be deleted with the command

**TAB ALL (OFF)** i,j,k,..

where i,j, and k are component ID numbers. If the tables are deleted, individual tables can be requested with the following commands:

<u>Command</u>	<u>Contents of Table</u>
<b>TAB ACT</b> i,j,k,..	activity coefficients
<b>TAB FUG</b> i,j,k,..	standard state fugacities, vapor phase fugacities, liquid phase activity coefficients
<b>TAB K</b> i,j,k,..	K-values
<b>TAB T</b> i,j,k,..	bubble point temperatures
<b>TAB P</b> i,j,k,..	bubble point pressures

Alternatively, individual tables can be deleted with the OFF option.

**TAB ACT (OFF)** i,j,k,..

**TAB K (OFF)** i,j,k,..

*Example 1.* VLE data has been reduced for the components, water (62) and ethanol (1012). The optional tables are not desired.

**TAB ALL (OFF)** 62, 1012.

*Example 2.* VLE data has been reduced for the components water (62) and ethanol (1012). Print only tables for bubble

## Chapter 16

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point temperatures, pressures, vapor compositions, and fugacities. The commands are:

**TAB T** 62, 1012.  
**TAB P** 62, 1012.  
**TAB ALL (OFF)** 62, 1012.  
**TAB FUG** 62, 1012.  
**TAB Y** 62, 1012.

or alternatively,

**TAB K (OFF)** 62,1012  
**TAB ACT (OFF)** 62,1012

### **ChemTran: Vapor Phase Fugacity Commands**

#### **ChemTran: Chemical Theory Vapor Phase Fugacity**

##### **CHEmical THEory VAPor**

This command is used to specify a vapor phase fugacity method that accounts for vapor phase association. This method will model the chemical equilibrium between dimers that form in the vapor phase when strongly associating chemical species are present. This option uses both the method of Hayden and O'Connell and Nothnagel's formulations. Please see [ChemTran: Vapor Phase Association Commands](#) for required parameters definition when CHE THE VAP is used in both ChemTran and DESIGN II.

#### **ChemTran: Hayden O'Connell Vapor Phase Fugacity**

##### **HADen OCOnnell VAPor**

This command is used to specify a vapor phase fugacity method that accounts for vapor phase association. This method uses a virial equation to calculate the vapor phase fugacity and calculates equilibrium constants for the formulation of dimers.(Hayden,J.G. and O'Connell,J.P., Ind. Eng. Chem. Process. Des. Dev., 14(3), 1975). Please see [ChemTran: Vapor Phase Association Commands](#) for required parameters definition when HAD OCO VAP is used in both ChemTran and DESIGN II.

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## **ChemTran: Selecting Correlations for Mixture Data**

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ChemTran is designed to offer an efficient way of preparing mixture property data for process simulations done with DESIGN II. This program contains options for many different K-values and enthalpy data systems. Many of these systems can generate K-values and enthalpies from pure component data treated in ChemTran. Others require the analysis experimental mixture data.

Several methods for treating mixture data are contained in ChemTran. When little mixture data is available it may be possible to use UNIFAC or regular solution theory to estimate mixture behavior. If this is not feasible it may then be necessary to use the IDEALK option. When more data exist extensive correlation capabilities can be used to regress excess enthalpy and almost any form of phase equilibrium data. For example, Vapor-Liquid Equilibrium data (VLE), Liquid-Liquid Equilibrium data (LLE), VLLE data and LLE data can be regressed simultaneously or independently. This is an important tool for obtaining good thermodynamic models of multi-phase systems. Once the data analysis is completed, the results can be transferred directly to DESIGN II using the FILE statements discussed in *ChemTran File Access Commands*.

This section presents some background material on the treatment of mixtures and the types of data which may be entered into ChemTran. The topics covered are:

### **ChemTran: Classification of Mixtures**

In a mixture of "N" components there are always "N(N-1)/2" unique binary pairs and the interactions between each pair must be accounted for in a simulation. For example, if the mixture consists of four components, A,B,C, and D, there are six unique binary pairs: A+B,A+C,A+D,B+C,B+D, and C+D. Depending on the types of components, each interaction can be specified as ideal, regular, or with mixture data. The most accurate specification is with mixture data, but this may not be available or necessary. Simulation of mixture properties in ChemTran relies on the specification of interaction constants for each unique pair of species in a mixture. These constants may be entered into the program directly in the form of VAN Laar, MARgules, RENon, WILson, UNIQUAC, PENg-Robinson, APIISOAVE, SOAVE, or infinite dilution activity coefficients. In addition, there are options to specify the interactions as ideal or regular (the SCAtchard-Hildebrand option). In some mixtures, either all or part of the binary interactions may be treated as ideal. This approximation is usually adequate if:

1. The chemicals are similar in structure, i.e., members of a homologous series. (e.g. butanol and pentanol)
2. They are of similar size. Mixtures of isomers are a good example of ideal solutions. The approximation of ideality would not apply if two similar chemicals are being separated.

Few typical behavior of component interactions are listed below:

#### **ChemTran: Regular Interactions**

When interactions between species are somewhat stronger than would be covered by the ideal approximations, the regular solution approximation may be applicable. This specification works fairly well for members of Group I and II (non-polar



components) in the Table 5.1 below. It is somewhat risky to specify interactions as regular if they are weak enough to be classified as ideal. Generally, this approximation should be used for non-polar chemicals. It does not work well for fluorocarbons.

Table 5.1. Classes of Chemicals

No.	Type	Examples
I	saturated hydrocarbons	n - C <sub>7</sub> H <sub>14</sub> , iso - C <sub>7</sub> H <sub>14</sub>
II	non-polar	CCl <sub>4</sub> , benzene, but not fluorocarbons
III	polar and non-associating; chlorinated hydrocarbons	CH <sub>3</sub> - C-CH <sub>3</sub> , CHCl <sub>3</sub> , $\begin{array}{c} \parallel \\ \text{O} \\ \text{CH}_2 - \text{CH}_2 \end{array}$ $\text{O} \left( \quad \quad \right) \text{O}, \text{CH}_3, \text{NO}_2$ $\text{CH}_2 - \text{CH}_2$
IV	polar and associating or hydrogen bonding, such as alcohols, phenols, acids, amines, glycols	H <sub>2</sub> O, CH <sub>3</sub> HO $\begin{array}{c} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\   \quad \quad   \\ \text{OH} \quad \quad \text{OH} \end{array}$

### ChemTran: Strong Interactions

When mixtures contain molecules from Groups III and IV, interactions become very strong and it may be necessary to enter either experimental data for correlation or data in the form of constants. *ChemTran: Correlating Mixture Data* describes in detail procedures for correlating V-L-E data. Because of the nature of the substituents, mixtures normally occurring in hydrocarbon processing will require less data than those which occur in chemical processing.

### ChemTran: Examples of Chemical Systems

Consideration must be given to the type of system and the process goals to be met in order to determine which interaction specifications are applicable for a simulation. The following examples will provide some guidelines in making these decisions.

### ChemTran: Hydrocarbon Processing

A classic example in hydrocarbon processing is the separation of C paraffins, olefins and diolefins by extract distillation using furfural as a solvent. In this case, some binary data would be needed to predict vapor liquid equilibrium in multi-component mixtures. For example, if the following components are in a mixture,

n-butane 1-butene 1,3-butadiene furfural

the possible binary interactions are:

- |                   |               |
|-------------------|---------------|
| A. n-butane:      | 1-butene      |
| B. n-butane:      | 1,3-butadiene |
| C. n-butane:      | furfural      |
| D. 1-butene:      | 1,3-butadiene |
| E. 1-butene:      | furfural      |
| F. 1,3-butadiene: | furfural      |

Interactions between hydrocarbons (A,B,D,) are only slightly non-ideal and will be predicted adequately by the internal data system of other WinSim programs. But the interactions between furfural and the hydrocarbons (C,E,F,) are highly non-ideal and cannot be predicted with adequate accuracy by state-of-the-art methods.

### ChemTran: Chemical Processing

An example of a classic chemical processing problem is the preparation of absolute alcohol by azeotropic distillation with benzene. In this mixture, the components are:

Ethanol Water Benzene

which gives the following binary interactions:

Ethanol - Water Ethanol - Benzene Water - Benzene

All three of the binary interactions are highly non-ideal and will require user-provided information to predict the behavior of the ternary system.

### ChemTran: Complex Mixtures

The type of data system used to specify the interaction parameters depends on the types of separations desired as well as the types of species. Thus, in a mixture consisting of:

acetone n-butane 2-butene 2-butene

where separation of the hydrocarbons from acetone is the goal, a specification of ideal for the hydrocarbon interactions might be adequate. However, this would not be true for a mixture of:

n-butane 1-butene 2-butene

## Chapter 16

where the goal is to separate the hydrocarbons from each other. This separation depends explicitly on the interaction between the hydrocarbons and it is crucial that they be represented accurately in the simulation.

### **ChemTran: V-L-E Data Systems**

ChemTran is designed not only to simulate vapor-liquid or liquid-liquid equilibria for mixtures, but also to set up data systems for these simulations in other programs. All three functions of ChemTran - the data base, the pure component properties generator and the correlation capabilities may be used in setting up the data systems for a simulation. Although the program removes the difficulties in these calculations, it is helpful to have some familiarity with the procedures. The following discussion outlines the concepts and types of data required for analysis of mixture data.

There are two basic approaches to simulating vapor-liquid or liquid-liquid equilibrium. The first method uses activity coefficient correlations for the liquid phase and an equation of state for the vapor phase. The second uses an equation of state to represent both the liquid and vapor phases.

### **ChemTran: Activity Coefficient Correlations**

In the activity coefficient approach, mixture vapor-liquid or liquid-liquid equilibrium involves dealing with some combination of the following quantities (for a component  $i$ ):

$Y_i$ ,	the vapor phase concentrations;
$X_i$ ,	the liquid phase concentrations;
$P$ ,	the pressure of the system;
$T$ ,	the temperature of the system;
$\phi_i$ ,	the vapor phase fugacity coefficients;
$f_i^{ss}$ ,	the standard state liquid phase fugacities;
$\gamma_i$ ,	the liquid phase activity coefficients;

The primary relationships between these variables are

$$Y_i \phi_i P = X_i f_i^{ss} \gamma_i$$

for vapor-liquid equilibrium and for the liquid phase,

$$X_i^{(1)} \gamma_i^{(1)} \quad (\text{liquid phase 1}) =$$

$$X_i^{(2)} \gamma_i^{(2)} \quad (\text{liquid phase 2}).$$

The quantities  $\phi_i$ ,  $f_i^{ss}$ , and  $\gamma_i$  provide connecting links between the variable  $T$ ,  $P$ ,  $X_i$ , and  $Y_i$ . ChemTran contains all of the correlations and algorithms necessary for calculating these links.

### **ChemTran: Activity Coefficients $\gamma^i$ from Data**

Activity coefficients,  $\gamma^i$ , are obtained from either the RENon, WILson, or UNIQUAC correlation equations for mixture data. The type of equation used is an option specified by the user. They require that a set of interaction parameters be entered into the program for each binary pair which is treated as strongly interacting. For ideal and regular interactions, interaction parameters are determined by ChemTran. When interaction parameters are not available, mixture data must be entered and analyzed as described in *ChemTran: Correlating Mixture Data*.

All of the types of interaction parameters which can be processed by ChemTran are summarized in *ChemTran: Binary Interaction Coefficients Table*.

### **ChemTran: Activity Coefficient at Infinite Dilution**

An activity coefficient at infinite dilution is defined as the limiting value of the activity coefficient of a component as its mole fraction approaches zero, that is:

$$\gamma_1^\infty = \lim_{x_1 \rightarrow 0} \gamma_1$$

$$\gamma_2^\infty = \lim_{x_2 \rightarrow 0} \gamma_2$$

Such values are subject to direct measurement and can be obtained in the dilute regions. Also, some methods of predicting behavior of highly non-ideal solutions, such as those of Pierotti, Deal and Derr, I&E, Vol. 51, 95 (1959), result in the prediction of infinite dilution coefficients. Values of  $\gamma_1^\infty$  and  $\gamma_2^\infty$  are entered on an ACT command and converted directly to WILson, RENon, or UNIQUAC constants by the program.

### **ChemTran: Activity Coefficients From UNIFAC Correlation**

UNIFAC is a powerful correlation for liquid phase activity coefficients applicable to non-ideal systems (e.g., alcohols, aldehydes, ketones, H<sub>2</sub>O etc.). Experimental data are not required for its application. It was developed by J.M. Prausnitz, et al. in 1975 and has since been applied to most of the world's literature (about 75%) on vapor-liquid equilibrium data by A. Fredenslund, et al.

This correlation takes a vastly different approach from previous correlations. Instead of modeling a mixture as a set of chemicals, it models it as a set of substituent groups which make up those chemicals. For example, a mixture of propanol and methyl-ethyl-ketone is pictured as a combination of CH<sub>3</sub>, CH<sub>2</sub>OH, and C=O groups. The model then uses group interaction parameters to describe interactions between groups and to predict K-values. Since there are only 25 to 40 different groups, as compared to thousands of chemicals, these group interactions can be used to predict K-values for literally millions of different chemical mixtures.

DESIGN II has combined this powerful correlation with its Data Base to provide you the capability of predicting K-values for an almost endless variety of non-ideal mixtures. We have put in our database the necessary group information to predict K-values for almost any combination of over 600 chemicals. There will be some exceptions because not all of the group interaction parameters have been developed. These will be added as they become available.

UNIFAC can be used directly in DESIGN II using the K-value option:

### UNIFACK

in the GENERAL section of DESIGN II.

In ChemTran the UNIFAC correlation can be combined with an existing data to obtain binary interaction parameters for WILson, RENon, or UNIQUAC equations. This accomplished with the command:

**ACT (UNIFAC) i,j = T**

where i and j are the component ID numbers and T is an average temperature for the mixture.

For components not in the database, a UNIFac structure description may be entered. This is not necessary if the STRUcture command has been entered. See *ChemTran: Using the Structure Command to Define a Custom Component* for details.

If UNIFAC is not applicable for a particular combination of chemicals, the program will not execute any calculations; your output will list the combination(s) of components in your system not presently predicted by UNIFAC. There are only a few restrictions which should be adhered to for the UNIFAC K-value option:

1. It should be used only for pressures of about 1-3 atm.
2. It should be used only for temperatures from about 30-125 degrees C.
3. All components in the mixture should be condensable (e.g., no CO, CO<sub>2</sub>, N<sub>2</sub>, etc.)

Within these restrictions, UNIFAC can be applied to mixtures consisting of two to three chemicals selected from the following classifications:

hydrocarbons	ether
alcohols	aromatics
ketones	chlorinated hydrocarbons
aldehydes	carbon disulfide
amines	organic nitrates
water	

The UNIFAC K-value method should not be used as a replacement for data. Since it is applicable to such a tremendous variety of systems it may not be as accurate for a particular system as actual data. However, it is an extremely useful tool for checks of processes when you do not have time to collect data, for preliminary process calculations, or for systems where no data exist. The accuracy of UNIFAC will, of course, vary from system to system. However, Fredenslund has demonstrated that for bubble point calculations on a variety of systems and conditions; errors in T will be in the range of 0 to approximately 2 degrees K and errors in Y will be in the range .005 to approximately .07. Checks on UNIFAC predictions for specific systems can be made with dew or bubble point calculations in DESIGN II.

### ChemTran: Equations of State

The equation of state approach to simulation of vapor-liquid equilibrium relies on the fundamental relationship

$$Y_i \phi_i^{\text{vap}}(T, P, Y_i, A, B) = X_i \phi_i^{\text{liq}}(T, P, X_i, A, B),$$

where

$\phi_i^{\text{vap}}$  = fugacity coefficient of component i in the vapor

Y = mole fraction of component i in the vapor

$\phi_i^{\text{liq}}$  = fugacity coefficient of component i in the liquid

$X_i$  = mole fraction of component i in the liquid

Both  $\phi_i^{\text{vap}}$  and  $\phi_i^{\text{liq}}$  are calculated from an equation of state. Parameters A and B are used to adjust the fugacity equality to fit experimental data. The parameter B is used to account for temperature dependence.

### ChemTran: Peng Robinson, APISOAVE, Soave

$\phi_i$  from PENg-Robinson, APISOAVE and SOAVE Equations

## Chapter 16

The PENg Robinson and SOAVE equations provide an acceptable simulation of K-values for mixtures of low molecular weight hydrocarbons with default interaction parameters. These interactions would include those among hydrocarbons from weight hydrocarbons with default interaction parameters. These interactions would include those among hydrocarbons from CH<sub>4</sub> up to around pentane or hexane. Of course, the K-values could be made more accurate by entering V-L-E data.

If the mixture contains heavier hydrocarbons, unsaturated hydrocarbons, or inorganic gases such as H<sub>2</sub>S, CO<sub>2</sub>, N<sub>2</sub>, COS, and O<sub>2</sub> then it may be necessary to enter VLE data. Also entry of VLE data is strongly suggested for separation of two similar chemicals, for example, in an ethane-ethylene or propane-propylene splitter.

In general, these equations are preferable to WILson or RENon for high pressure systems (greater than 10 to 15 atm). This option is normally not used in systems of strongly interacting chemicals such as alcohols, water amines, glycols, etc. In these cases, WILson or RENon would be the better choice

### ChemTran: Modified Peng Robinson Equation of State

Choosing an appropriate thermodynamic method to adequately predict vapor liquid equilibria for high pressure non-ideal systems has in the past presented difficult trade-offs. An activity coefficient method can model liquid phase behavior well but does a poor job in the vapor phase, conversely, an equation of state method can predict the vapor phase well but does a poor job modeling non-ideal liquid phases. Making a choice has always been a compromise.

This new method is applicable to non-ideal chemical systems at high pressure. Its advantages are that it has improved ability to predict vapor pressures for polar and associating compounds and an improved ability to regress VLE data.

A new equation of state has been implemented in the DESIGN II and ChemTran programs for the modeling of non-ideal chemical systems at pressures higher than those for which the vapor phase can be assumed to be ideal. This equation of state is intended for determining both liquid and vapor phase fugacities and is an alternative to the mixed K-value models which employ an activity coefficient model in conjunction with a standard state fugacity correlation for determining liquid and vapor phase fugacity coefficients.

The Modified Peng-Robinson correlation is an equation of state that predicts the liquid phase with the accuracy of the activity coefficient method. This method is a ChemShare modified Peng-Robinson equation of state based on the work of Stryjek et al. (1).

Their work consisted of two modifications to the standard Peng-Robinson formulation. The first modification is to the attractive energy term of the Peng-Robinson equation for pure components. The modification is obtained by enhancing the temperature dependence of the term,  $\alpha$ , which multiplies the attractive energy parameter, a.

The Stryjek Modified Peng-Robinson attractive energy term is

$$\alpha = [1 + K(1 - Tr^{0.5})]^2$$

ChemShare determined that there are regions of the phase map for which the Stryjek modification of the Peng-Robinson equation is significantly less accurate than the standard Peng-Robinson equation. ChemShare, therefore, derived additional proprietary modifications to overcome these inaccuracies.

The ChemShare implementation defines

$$K = f + (K_0, K_1, K_2, K_3, \text{Temperature})$$

where  $K_0$  is

$$K_0 = 0.37464 + 1.54226 \omega - 0.26992 \omega^2$$

and  $K_1$ ,  $K_2$  and  $K_3$  are terms calculated from a vapor pressure data regression.

Owing to these proprietary modifications, the Kappa Parameters published by Stryjek and Vera are not applicable. The user must regress pure component vapor pressure data with ChemTran to calculate the kappa parameters for each component. If pure component vapor pressure data is not regressed, the equation of state will default to the standard Peng-Robinson equation.

In addition to the modification to the attractive energy term, a new composition dependent mixing rule has been added for this equation of state. This requires the correlation of two interaction parameters per binary pair. For strongly non-ideal systems, this new mixing rule can result in an order of magnitude improvement in the fit of vapor-liquid equilibrium (VLE) data.

The modified Peng-Robinson equation can be used with either of two binary mixing rules. The first mixing rule is the standard binary mixing rule presented in any thermodynamic text. The new mixing rule is similar in form to the Margules activity coefficient model and takes its name from the equation. The attractive energy term is defined as:

$$a\alpha_{ij} = (1 - x_i k_{ij} k_{ji}) \sqrt{(a\alpha)_i (a\alpha)_j}$$

<sup>1</sup> Stryjek, R. and Vera, J.H., Canadian Journal of Chemical Engineering, vol. 64, 1986

### ChemTran: MARGules Constants

Margules constants are defined by the equations

$$\log_{10} \gamma_1 = X_2^2 \{A_{12} + 2X_1 (A_{21} - A_{12})\}$$

$$\log_{10} \gamma_2 = X_1^2 \{A_{21} + 2X_2 (A_{12} - A_{21})\}$$

for a binary system of components 1 and 2. These parameters are converted either to **WILSON**, **RENon**, or **UNIQUAC** coefficients, depending on the option chosen.

### ChemTran: Liquid Activity Coefficient Correlations

One approach to simulating vapor-liquid /liquid-liquid equilibrium is to use activity coefficient correlations for the liquid phase and an equation of state for the vapor phase. Some of the liquid phase activity coefficient correlations are listed below:

#### ChemTran: RENon Equations

$$\ln(\gamma_i) = \frac{\sum_{j=1}^n x_j \tau_{ji} G_{ji}}{\sum_{k=1}^n x_k G_{ki}} + \sum_{j=1}^n \frac{x_j G_{ij}}{\sum_{k=1}^n x_k G_{kj}} \left( \tau_{ij} - \frac{\sum_{m=1}^n x_m \tau_{mj} G_{mj}}{\sum_{k=1}^n x_k G_{kj}} \right)$$

$$G_{ij} = \text{Exp}(-C_{ij} \tau_{ij})$$

$$\tau_{ij} = (A_{ij}/RT) + B_{ij, \tau_{ij}}$$

$$\tau_{ji} = (A_{ji}/RT) + B_{ji, \tau_{ji}}$$

where  $A_{ij} = (g_{ij} - g_{ji})$ ;  $A_{ji} = (g_{ji} - g_{ij})$ ;  $B_{ij, \tau_{ij}} = B_{ji, \tau_{ji}} = 0$  (most cases)

and  $C_{ij} = C_{ji}$  (scaling parameter typically 0.2)

and n is the number of components. The B constants will be zero in most cases. ChemTran uses these equations directly for user entered RENon constants.

#### ChemTran: UNIQUAC Equations

UNIQUAC constants are defined by:

$$\ln \gamma_i = \ln \frac{\psi_i}{x_i} + 5q_i \ln \frac{\theta_i}{\psi_i} + l_i - \frac{\psi_i}{x_i} \sum_{j=1}^m (x_j l_j) + q_i \left\{ 1 - \ln \left( \sum_{j=1}^m \theta_j \tau_{ji} \right) - \frac{m}{j=1} \left( \frac{\theta_j \tau_{ij}}{\sum_{k=1}^m \theta_k \tau_{kj}} \right) \right\}$$

where

$$l_j = 5(r_j - q_j) - (r_j - 1)$$

and also  $5 = Z/2$  where Z is lattice coordination number set equal to 10.

Segment Fraction: 
$$\psi_i = \frac{r_i x_i}{\sum_{i=1}^m r_i x_i}$$

Area Fraction: 
$$\theta_i = \frac{q_i x_i}{\sum_{i=1}^m q_i x_i}$$

$$\tau_{ji} = \text{Exp} \left( - \left( \frac{A_{ji}}{RT} + B_{ii} \right) \right)$$

- m is the number of components.
- r and q are volume and surface area parameters respectively that are unique for each species.

The B constants will be zero in most cases. ChemTran uses these equations directly for user entered UNIQUAC constants.

#### ChemTran: VAN Laar Equations

Constants for the Van Laar equations describing an interaction between components 1 and 2 are defined by

## Chapter 16

$$\log_{10} \gamma_1 = A_{12} X_2^2 / (A_{12} X_1 / A_{21} + X_2)^2$$

and

$$\log_{10} \gamma_2 = A_{21} X_1^2 / (X_1 + A_{21} X_2 / A_{12})^2$$

These constants are converted to WILson, RENon, or UNIQUAC constants in ChemTran.

### ChemTran: WILson Equations

For a mixture of m chemicals, the WILson correlation equations are:

$$\ln \gamma_k = 1 - \ln \sum_{j=1}^m X_j \Lambda_{kj} - \sum_{j=1}^m \frac{X_j \Lambda_{jk}}{\sum_{j=1}^m X_j \Lambda_{ij}}$$

$$\Lambda_{ij} = \frac{V_j(T)}{V_i(T)} \exp \left( - (A_{ij} X_i / RT + B_{ij}) \right)$$

where V (T) is the liquid volume for component i. These equations are used directly by ChemTran when WILson constants are entered on a WIL statement in *ChemTran: Wilson Parameters*.

### ChemTran: Vapor Phase Fugacity Coefficients

$\phi_i$  and  $f_i^{ss}$

Vapor phase fugacity coefficients are evaluated from pure component data, either from the Data Base or generated, using the Redlich-Kwong equation of state. Standard state liquid phase fugacities are calculated from the equation

$$f_i^{ss} = \phi_i^{sat} \text{EXP} \{ V_i^{liq} (P - P_i^{sat}) / RT \}$$

where

$\phi_i^{sat}$  is the vapor phase fugacity coefficient for pure component i;

$P_i^{sat}$  is the saturated liquid vapor pressure; and

$V_i^{liq}$  is the saturated liquid volume of pure component i.

As this equation indicates, these calculations require pressure and volume data. This is supplied automatically for components in Data Base. For other components, or to override Data Base values, a V-T and P-T card may be used to supply liquid volume and vapor pressure data. As of  $\phi_i$ ,  $\phi_i^{sat}$  is evaluated using the Redlich-Kwong equation of state. No special provision is made for entering  $f_i^{ss}$  for non-condensable components. These components are usually handled adequately by permitting ChemTran to provide default values.

### ChemTran: Binary Interaction Coefficients Table

Table 5.2. - Binary Interaction Constants

Parameter Type	Parameters	Defaults	Command	Comments
Infinite dilution	$\gamma_i^\infty, \gamma_j^\infty$	- -	<b>ACT</b>	converted automatically to WILson, RENon, or UNIQUAC constants as specified by the K-value option.
Margules constants	$A_{ij}, A_{ji}$	- -	<b>MAR</b>	entered for binary pair i and j, converted to WILson, RENon, or UNIQUAC constants as specified by the K-value option.
Renon constants	$A_{ij}, A_{ji},$ $B_{ij}, B_{ji},$ $C_{ij}, C_{ji}$	$A_{ij}=A_{ji}=0$ $B_{ij}=B_{ji}=0$ $C_{ij}=C_{ji}=0.2$	<b>REN</b>	Used directly or B,B $C_{ij}, C_{ji}, C_{ij}=C_{ji} = 0.2$ fitting V-L-E data; for use with the RENon K-value option.
Van Laar constants	$A_{ij}, A_{ji},$		<b>VAN</b>	Entered for binary pair i and j, converted to WILson, RENon, or UNIQUAC constants as specified by the K-value option.
Wilson constants	$A_{ij}, A_{ji},$	$A_{ij}=A_{ji}=0$	<b>WIL</b>	used directly or for V-L-E data; use with the WILson K-value option.
UNIQUAC constants	$A_{ij}, A_{ji},$ $B_{ij}, B_{ji},$	$A_{ij}=A_{ji}=0$ $B_{ij}=B_{ji}=0$	<b>UNIQUAC</b>	used directly or for estimates in fitting V-L-E data ; use with the UNIQUAC K-value option.
Peng-Robinson	$A_{ij}, B_{ij}$	$A_{ij}=0$ $B_{ij}=0$	<b>PEN</b>	used directly or constant for estimates in fitting V-L-E data.
APISOave	$A_{ij}, B_{ij}$	$A_{ij}=0$	<b>APISOAVE</b>	used directly or for constants estimates in fitting V-L-E data; use with the APISOAVE K-value option (See <i>Thermodynamics: Table 1. APISOAVEK Interaction Parameter List</i> for binary

pairs for which A will not be zero.)

Soave Constants	$A_{ij}, B_{ij}$	$A_{ij}=0$ $B_{ij}=0$	<b>SOAVE</b>	used directly or for in fitting V-L-E data; use with the SOAVE K-value option.
Modified Peng Robinson	$A_{ij}, A_{ji}$ $B_{ij}, B_{ji}$	$A_{ij}=A_{ji}=0$ $B_{ij}=B_{ji}=0$	<b>MOD PEN</b>	used directly or for data; for use with MOD PEN K

### ChemTran: Enthalpy Data Systems

Most process simulations require, in addition to data systems for K-values, the specification of a data system for mixture enthalpies. ChemShare programs contain several systems for enthalpies. Many of these are predictive and do not require enthalpy data; however, for a few of the systems, it is necessary to enter enthalpy data. The predictive systems do require the pure component data provided by ChemTran when enthalpy data is required. ChemTran provides for the preparation and examination of this data for use in the simulation programs.

### ChemTran: LATent Heat Data

Sometimes latent heat data as a function of temperature is available in the absence of direct liquid and vapor enthalpy data. This method uses this data and an internal data system to calculate liquid enthalpy data from predicted vapor enthalpies.

### ChemTran: TABular Vapor and Liquid Enthalpy

This system assumes that a stream molar enthalpy is equal to the molar average of the enthalpy data which is entered. Thus, if partial molar enthalpies are entered, the stream enthalpy is calculated rigorously. If pure component enthalpies are entered, then the calculation assumes an ideal solution with no heat of mixing. **When this system is used, enthalpy data for all components in both vapor and liquid must be entered.**

### ChemTran: Excess Enthalpy Data

**EXC LAT**  
**EXC TAB**

Excess enthalpy data may be used in addition to pure component liquid and vapor enthalpy data for a rigorous calculation of stream enthalpies. This calculation employs the relationship:

$$\underline{H}_m(T,P,X) = H^e(T,P,X) + \sum_{i=1}^n X_i \underline{H}_i(T,P)$$

where

$\underline{H}_m$  is the molar enthalpy of mixture;

$\underline{H}_e$  is the excess molar enthalpy ; and

$\underline{H}_i$  is the molar enthalpy of pure component i.

When excess enthalpy data is entered with the HE-T-X command, it is correlated to the NRTL (RENon) excess enthalpy equations. If no excess enthalpy data is available, this data system can still be used by reducing V-L-E data using the *ChemTran: RENon Equations*. When this is done the resulting binary interaction coefficients may be used in the NRTL excess enthalpy equations.

### ChemTran: Table for Enthalpy Data Systems

**Table 5.3. Enthalpy Data Systems**

<b>System Name</b>	<b>Data Required</b>	<b>Data Input Statement</b>
<b>TABular</b>	pure component vapor and liquid enthalpy data, or partial molar enthalpy data	<b>HL-T</b> and <b>HV-T</b>
<b>LATent heat</b>	pure component latent heat data	<b>L-T</b>
<b>EXC LAT</b> <b>EXC TAB</b>	excess enthalpy data or V-L-E data with Renon option	<b>HE-T-X</b> <b>T-P-Y-X</b> or <b>T-Y-X</b> or <b>P-Y-X</b> or <b>T-P-X</b> or <b>T-X</b> or <b>P-X</b> OR <b>T-X-X</b>
any enthalpy option used with solid components	solid enthalpy data	<b>HS-T</b>

The data systems requiring enthalpy data are summarized in the above table. Only pure component data is required for the standard and latent heat systems. Entry of this data and the corresponding curve fitting procedures has been presented in *ChemTran: Latent Heat*, *ChemTran: Excess Enthalpy Commands*, and *ChemTran: Supplementary Commands*.

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**ChemTran: Phase Equilibrium Data Entry**


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**ChemTran: Pressure-Liquid Phase Equilibrium Data**

**P - X** (units, option) i, j, k, = T, P<sub>1</sub>, X<sub>1i</sub>, X<sub>1j</sub>, ..., P<sub>2</sub>, X<sub>2i</sub>, X<sub>2j</sub>, ...

This command is used to enter pressure versus liquid phase concentration at a constant temperature for a system composed of *n* components. Component ID numbers are entered as shown for i, j, k, ... The data must be for liquid-vapor systems and **not** liquid-liquid systems.

**P-X** data for a binary pair would be entered as follows:

**P - X** (units) i, j = T, P<sub>1</sub>, X<sub>1i</sub>, P<sub>2</sub>, X<sub>2i</sub>, P<sub>3</sub>, X<sub>3i</sub>

**NOTE:** ChemTran automatically calculates  $X_j = 1 - X_i$

**NOTE:** The program assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

**Example 1.** **P-X** (MMHG,C) 202, 205 - 55., 300., 0.1, 428., .2, 555., .4, 709., 0.7, 897., .915,

The data is for the binary system of components 202 and 205 at T - 55.0 °C and

<b>P, mm Hg</b>	<b>mol fr. X<sub>202</sub></b>	<b>mol fr. X<sub>205</sub></b>
300.0	0.1	0.9
428.	0.2	0.8
555.0	0.4	0.6
709.00	0.7	0.3
897.0	0.915	0.085

If the **GEN VLE** option is specified, the **P-X** command does not regress data, rather it is used to generate vapor phase compositions at the specified liquid phase composition. If **P-Y** is specified then liquid phase composition will be calculated for the specified vapor phase composition.

**ChemTran: Pressure-Vapor-Liquid Equilibrium Data**

**P - Y - X**(units) i, j, k, ... = T, P<sub>1</sub>, Y<sub>1i</sub>, Y<sub>1j</sub>, ..., X<sub>1i</sub>, X<sub>1j</sub>, ..., P<sub>2</sub>, Y<sub>2i</sub>, Y<sub>2j</sub>, ..., X<sub>2i</sub>, X<sub>2j</sub>,

This command is used to enter pressure versus vapor and liquid compositions for a mixture of *n* components, where i, j, k represent component ID numbers. The data are measured at a constant temperature, T. You may also enter the concentration data with liquid first, vapor second. The form of the command would then be

**P - X - Y**(units) i, j, k, ... = T, P<sub>1</sub>, X<sub>1i</sub>, X<sub>1j</sub>, ..., Y<sub>1i</sub>, Y<sub>1j</sub>, ...

**NOTE:** For an *n* component system, you enter *n*-1 values for Y and X. ChemTran automatically calculates the values for the last component.

ChemTran assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units option for this command.

**Example 1.** **P-Y-X** (MMHG, C) 202, 203, 205 = 55.0, 665.3, .188, .196, .512, .139, 690.3, .198, .396, .513, .262, 689.7, .198, .396, .511, .263, 706.5, .195, .592, .507, .373, 711.2, .359, .323, .540, .254,

In this example, data is being entered for a three component system at a constant temperature of 55.0 °C. The component ID numbers are 202, 203, and 205; the VLE data is

<b>P, mm of Hg</b>	<b>mol fr. Y<sub>202</sub></b>	<b>mol fr. Y<sub>203</sub></b>	<b>mol fr. X<sub>202</sub></b>	<b>mol fr. X<sub>203</sub></b>
665.3	0.188	0.196	0.512	0.139
690.3	0.198	0.396	0.513	0.262
689.7	0.198	0.396	0.511	0.263
706.5	0.195	0.592	0.507	0.373
711.2	0.359	0.323	0.540	0.254

**ChemTran: Pressure-Vapor-Liquid-Liquid Equilibrium Data**

**P - Y - X - X**(units) i, j, k, ... = T, P<sub>1</sub>, Y<sub>1i</sub>, Y<sub>1j</sub>, ..., X<sub>1i</sub><sup>1</sup>, X<sub>1j</sub><sup>1</sup>, ..., X<sub>1i</sub><sup>2</sup>, X<sub>1j</sub><sup>2</sup>, ..., P<sub>2</sub>, Y<sub>2i</sub>, Y<sub>2j</sub>, ..., X<sub>2i</sub><sup>1</sup>, X<sub>2j</sub><sup>1</sup>, ..., X<sub>2i</sub><sup>2</sup>, X<sub>2j</sub><sup>2</sup>

Isothermal data (at temperature T) for pressure versus the compositions of components in the vapor, liquid phase 1, and liquid phase 2 are entered with this command. Experimental data entered on this command must be for a mixture with three phases in equilibrium. **It should be used only with the UNIQUAC or RENON equation options.** The components in the system are i, j, k, etc. You may also enter liquid concentration data first, vapor second. The command then becomes



$$P - X - X - Y(\text{units})_{i,j,k,\dots} = T, P_1, X_{1i}^1, X_{1j}^1, \dots, X_{1i}^2, X_{1j}^2, \dots, Y_{1i}, Y_{1j}, \dots,$$

**NOTE:** For an  $n$  component mixture, you enter  $n-1$  values for  $Y$ ,  $X(\text{phase } 1)$  and  $X(\text{phase } 2)$ . ChemTran automatically calculates the values for the last component.

ChemTran assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units option for this command

**Example 1.** Enter the following data for a mixture of benzene, ethanol, and water measured at 65.9 °C with a vapor phase and two liquid phases. The component ID numbers are 40, 1012, and 62 respectively. (see *Database Components*).

P mm of Hg	vapor phase			Mole Fractions					
	Y <sub>1012</sub>	Y <sub>40</sub>	Y <sub>62</sub>	benzene phase			water phase		
				X <sub>1012</sub>	X <sub>40</sub>	X <sub>62</sub>	X <sub>1012</sub>	X <sub>40</sub>	X <sub>62</sub>
760	.241	.548	.211	.232	.664	.104	.225	.021	.754
760	.248	.543	.209	.281	.555	.164	.277	.048	.675

P-Y-X-X (MMHG,C) 1012, 40, 62=64.9,  
760., .241, .548, .232, .664, .225, .021,  
760., .248, .543, .281, .555, .277, .048,

### ChemTran: Temperature-Pressure-Liquid Equilibrium Data

$$T - P - X(\text{units})_{i,j,k,\dots} = T_1, P_1, X_{1i}, X_{1j}, \dots, T_2, P_2, X_{2i}, X_{2j}, \dots,$$

Temperature -pressure-liquid composition data for an  $n$  component mixture are entered with this command. The component ID numbers are represented by  $i,j,k$ .

**NOTE:** For an  $n$  component system, you enter  $n-1$  values for  $X$ . ChemTran automatically calculates the value for the last component.

**Example 1.**

T-P-X (C,ATM) 220,210 = 30., 1.340, .1564, 34., 1.896, .2007, 40., 2.789, .6098

The data entered for this binary system are mole fractions

T, °C Hg	P, atm	mol fr. X
30.0	1.340	.1564
34.0	1.896	.2007
40.0	2.789	.6098

### ChemTran: Temperature-Pressure-Vapor-Liquid Equilibrium Data

$$T - P - Y - X(\text{units})_{i,j,k,\dots} = T_1, P_1, Y_{1i}, Y_{1j}, \dots, X_{1i}, X_{1j}, \dots, T_2, P_2, Y_{2i}, Y_{2j}, \dots, X_{2i}, X_{2j}, \dots, T_3, P_3, Y_{3i}, Y_{3j}, \dots, X_{3i}, X_{3j}, \dots$$

This command is used to enter temperature-pressure-vapor phase composition-liquid phase composition for a multi-component mixture with components  $i,j,k,\dots$  represent component ID numbers.

You may also enter concentration data with liquid fraction first, then vapor fractions. The command would be written as follows:

$$T - P - X - Y(\text{units})_{i,j,k,\dots} = T_1, P_1, X_{1i}, X_{1j}, \dots, Y_{1i}, Y_{1j}, \dots$$

**NOTE:** For an  $n$  component mixture, you enter  $n-1$  values for  $Y$  and  $X$ . The program automatically calculates the values for the last component.

ChemTran assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

**Example 1.**

T-P-X Y (MMHG,C) 220,202 = 45., 250.73, .144, .0470, 72.8, 760., .4, .2,

The data entered in this example for components 220 and 202 are:

T, °C	P, mm Hg	mol fr. Y	mol fr. X
45.0	250.73	0.1444	0.0470
72.8	760.0	0.4000	0.2000

### ChemTran: Temperature-Pressure-Vapor Phase-Liquid Phase 1-Liquid Phase 2 Equilibrium Data

$$T - P - Y - X - X(\text{units})_{i,j,k,\dots} = T_1, P_1, Y_{1i}, Y_{1j}, \dots, X_{1i}^1, X_{1j}^1, \dots, X_{1i}^2, X_{1j}^2, \dots, T_2, P_2, Y_{2i}, Y_{2j}, \dots, X_{2i}^1, X_{2j}^1, \dots, X_{2i}^2, X_{2j}^2, \dots,$$

Mixture data which shows both the temperature and pressure dependence on the compositions of a vapor phase, liquid phase 1, and liquid phase 2 are entered with this command. Experimental data entered with this command must be for  $n$  component mixture with the three phases in equilibrium. It should be used only with the UNIQUAC or RENON equation options. The  $i,j,k$

## Chapter 16

represent the component ID numbers. You may reverse the order for concentration data. The command becomes:

$$T - P - X - X - Y \text{ (units)} i, j, k, \dots = T_1, P_1, X_{i1}^1, X_{j1}^1, \dots, X_{i1}^2, X_{j1}^2, \dots, Y_{i1}, Y_{j1}, \dots,$$

**NOTE:** For an  $n$  component mixture, you enter  $n-1$  values for  $Y, X$  (phase 1 and  $X$  (phase 2)). The program automatically calculates the values for the last component.

ChemTran assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

**Example 1.** Enter the following data for a mixture of benzene, ethanol, and water. The data is for a vapor phase in equilibrium with a benzene-rich liquid phase and a water-rich liquid phase. The component numbers are 40, 1012, and 62 respectively.

T	P	Mole Fractions								
		vapor phase			benzene phase			water phase		
(°C)	(mm of Hg)	$Y_{1012}$	$Y_{40}$	$Y_{62}$	$X_{1012}$	$X_{40}$	$X_{62}$	$X_{1012}$	$X_{40}$	$X_{62}$
67.0	760.	.019	.643	.248	.020	.963	.017	.048	.001	.951
66.0	760.	.160	.601	.239	.046	.933	.021	.077	.002	.921
64.9	760.	.241	.548	.211	.232	.664	.104	.225	.021	.754
67.0	760.	.019	.643	.248	.020	.963	.017	.048	.001	.951
66.0	760.	.160	.601	.239	.046	.933	.021	.077	.002	.921
64.9	760.	.241	.548	.211	.232	.664	.104	.225	.021	.754

T-P-Y-X-X (MMHG, C) 1012, 40, 62 =  
 67.0, 760., .109, .643, .020, .963, .048, .001,  
 66.0, 760., .160, .601, .046, .933, .077, .022,  
 64.9, 760., .241, .548, .232, .664, .225, .021,

### ChemTran: Temperature-Liquid Equilibrium Data

$$T - X \text{ (units, option)} i, j, k, \dots = P, T_1, X_{i1}, X_{j1}, \dots, T_2, X_{i2}, X_{j2}, \dots$$

This command is used to enter temperature-liquid phase composition data at constant pressure  $P$ . The data must be for liquid-vapor equilibria and **not** liquid-liquid equilibria.

**NOTE:** For an  $n$  component system, you enter  $n-1$  values for  $X$ . The program automatically calculates the value for the last component.

ChemTran assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

**Example 1.** T-X (K,MMHG) 203,206=760.,333.35,.045,331.40,.275,331.85,.667,

This command contains the following data:

Pressure = 760 mm HG

T, °K	X mol fr in liquid phase
333.35	0.045
331.40	0.275
331.85	0.667

If the **GEN VLE** option is specified, the **T-X** command does not regress data, rather it is used to generate vapor phase compositions at the specified liquid phase composition. If **T-Y** is specified then liquid phase composition will be calculated for the specified vapor phase composition.

### ChemTran: Temperature-Liquid-Liquid Equilibrium Data

$$T - X - X \text{ (units, option)} i, j, k, \dots = P, T_1, X_{i1}^1, X_{j1}^1, \dots, X_{i1}^2, X_{j1}^2, \dots, T_2, X_{i2}^2, X_{j2}^2, \dots$$

This command is used to enter data for an  $n$  component system with two liquid phases at constant pressure  $P$ , where  $i, j, k$  represent component ID numbers.

For the T-X-X command, the nomenclature is:

$X_{i1}^1$  in phase 1 at temperature  $T$

and

$X_{i1}^2$  in phase 2

Since this is a **partially miscible** system, the **Wilson** equation **cannot** be used for data reduction.

**NOTE:** For an  $n$  component system, you enter  $n-1$  values for  $X$ (phase 1) and  $X$ (phase 2). ChemTran automatically calculates values for the last component.

The program assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

*Example 1.* **T-X-X(MMHG,C)201,205=760.,20.,.998.,.0004,25.,.92.,.006,30.,.989.,.001,**

The data for this example at a constant pressure of 760 mmHg is

mole fraction comp. 201 in phase 1		X mole fraction comp. 201 in phase 2
T, °K	X <sub>201</sub> <sup>1</sup>	X <sub>201</sub> <sup>2</sup>
20.	.998	.0004
25.	.992	.0006
30.	.989	.0010

### **ChemTran: Temperature-Liquid Phase 1-Liquid Phase 2-Liquid Phase 3 Equilibrium Data**

**T - X - X - X**(units)<sub>i,j,k,...</sub> = P, T<sub>1</sub>, X<sub>1i</sub><sup>1</sup>, X<sub>1j</sub><sup>1</sup>, ..., X<sub>1i</sub><sup>2</sup>, X<sub>1j</sub><sup>2</sup>, ..., X<sub>1i</sub><sup>3</sup>, X<sub>1j</sub><sup>3</sup>, ..., T<sub>2</sub>, X<sub>2i</sub>, X<sub>2j</sub>, ..., X<sub>2i</sub><sup>2</sup>, X<sub>2j</sub><sup>2</sup>, ..., X<sub>2i</sub><sup>3</sup>, X<sub>2j</sub><sup>3</sup>, ...

Data for an *n* component mixture with three liquid phases in equilibrium at a constant pressure P, are entered with this command. There should not be a vapor phase present. **Only the RENON and UNIQUAC equation options can be used with this command.**

**NOTE:** For an *n* component mixture, you enter *n-1* values for X(phase 1), X(phase 2), and X(phase 3). ChemTran automatically calculates the values for the last component.

The program assumes concentrations are entered as **mol** fractions. For data in mass fractions, add, **MASFRAC** to the units options for this command.

*Example 1.* Correlate experimental data for a mixture with three liquid phases at equilibrium (no vapor phase) consisting of *n*-heptane, benzene, water and acetonitrile. The data is measured at 25 °C. The component ID numbers are 11, 40, 62, and 1003 respectively.

Mole Fractions Phase 1			
X <sub>11</sub>	X <sub>40</sub>	X <sub>62</sub>	X <sub>1003</sub>
.80931	.11575	.00000	.074940
.79905	.12619	.00000	.074760

Mole Fractions Phase 2			
X <sub>11</sub>	X <sub>40</sub>	X <sub>62</sub>	X <sub>1003</sub>
.00000	.00000	.76264	.23736
.00000	.00000	.77370	.22630

Mole Fractions Phase 3			
X <sub>11</sub>	X <sub>40</sub>	X <sub>62</sub>	X <sub>1003</sub>
.00606	.01244	.49913	.48237
.00824	.01719	.33640	.63817

**T-X-X-X** (MMHG, C) 11,40,62,1003=760.,  
25.,.80931,.11515,.0,0,0,.76264,.00606,.1244,.49913,  
25.,.79905,.12619,.0,0,0,.77370,.00824,.0719,.33640,

### **ChemTran: Temperature-Vapor-Liquid Equilibrium Data**

**T - Y - X**(units)<sub>i,j,k,...</sub> = P, T<sub>1</sub>, Y<sub>1i</sub>, Y<sub>1j</sub>, ..., X<sub>1i</sub>, X<sub>1j</sub>, ..., T<sub>2</sub>, Y<sub>2i</sub>, Y<sub>2j</sub>, ..., X<sub>2i</sub>, X<sub>2j</sub>, ..., T<sub>3</sub>, Y<sub>3i</sub>, Y<sub>3j</sub>, ..., X<sub>3i</sub>, X<sub>3j</sub>, ...

Data for temperature-vapor phase concentration-liquid phase concentration at constant pressures are entered on this command. The mixture consists of *n* components where *i,j,k...* represent component ID numbers. This data is treated in the same way as T-P-Y-X are P-Y-X data in the data reduction procedure.

You may also enter liquid concentration data first, then vapor concentration data. The command in this case becomes

**T - X - Y** (units)<sub>i,j,k,...</sub> = P, T<sub>1</sub>, X<sub>1i</sub>, X<sub>1j</sub>, ..., Y<sub>1i</sub>, Y<sub>1j</sub>, ..., T<sub>2</sub>, X<sub>2i</sub>, X<sub>2j</sub>, ..., Y<sub>2i</sub>, Y<sub>2j</sub>, ...

**NOTE:** For an *n* component system, you enter *n-1* values for Y and X. ChemTran automatically calculates values for the last component.

The program assumes concentrations are entered as **mol** fractions. For data in mass fractions, add **MASFRAC** to the units options for this command.

*Example 1.* Enter the following ternary data for components 200, 201 and 203 at a pressure of 760 mm of Hg:

## Chapter 16

T, °C	mol fr. Y <sub>200</sub>	mol fr. Y <sub>201</sub>	mol fr. X <sub>200</sub>	mol fr. X <sub>201</sub>
70.0	0.610	0.130	0.100	0.100
69.4	0.430	0.355	0.100	0.300
63.5	0.440	0.470	0.200	0.500
62.7	0.700	0.150	0.300	0.200
60.0	0.670	0.242	0.400	0.300
57.2	0.778	0.184	0.700	0.200

The command is as follows:

```
T-Y-X (MMHG,C) 200,201,203=760.,70.0,.61,.13,.1,.1,
69.4,.43,.355,.1,.3,63.5,.44,.47,.2,.5,
62.7,.7,.15,.3,.2,60.,.67,.242,.40,.3,
57.2,.778,.184,.7,.2,
```

### ChemTran: Temperature-Vapor Phase-Liquid Phase 1-Liquid Phase 2 Equilibrium Data

$T - Y - X - X$  (units)<sub>i,j,k,...</sub> = P, T<sub>1</sub>, Y<sub>1j</sub>, Y<sub>1j</sub>,..., X<sub>1j</sub><sup>1</sup>, X<sub>1j</sub><sup>1</sup>,..., X<sub>1j</sub><sup>2</sup>, X<sub>1j</sub><sup>2</sup>,..., T<sub>2</sub>, Y<sub>2j</sub>, Y<sub>2j</sub>,..., X<sub>2j</sub><sup>1</sup>, X<sub>2j</sub><sup>1</sup>,..., X<sub>2j</sub><sup>2</sup>, X<sub>2j</sub><sup>2</sup>,...

Isobaric data (at pressure P) showing the dependence of the temperature on the composition of the vapor phase, liquid phase 1, and liquid phase 2 are entered with this command. Experimental data entered on this command must be for a mixture with these three phases at equilibrium. **It should be used only with the UNIQUAC or RENON equation options.** The i,j,k, represent component ID numbers.

The order of vapor and liquid concentration data can be reversed. The command becomes

$T - X - X - Y$  (units)<sub>i,j,k,...</sub> = P, T<sub>1</sub>, X<sub>1j</sub><sup>1</sup>, X<sub>1j</sub><sup>1</sup>,..., X<sub>1j</sub><sup>2</sup>, X<sub>1j</sub><sup>2</sup>,..., Y<sub>1j</sub>, Y<sub>1j</sub>,..., T<sub>2</sub>, X<sub>2j</sub><sup>1</sup>, X<sub>2j</sub><sup>1</sup>,..., X<sub>2j</sub><sup>2</sup>, X<sub>2j</sub><sup>2</sup>,..., Y<sub>2j</sub>, Y<sub>2j</sub>,...

**NOTE:** For an *n* component mixture, you enter *n*-1 values for Y, X(phase 1), and X(phase 2). ChemTran automatically calculates the values for the last component.

The program assumes concentrations are entered as **mol fractions**. For data in mass fractions, add **MASFRAC** to units options for this command.

T (°C)	Mole Fractions								
	vapor phase			benzene phase			water phase		
	Y <sub>1012</sub>	Y <sub>40</sub>	Y <sub>62</sub>	X <sub>1012</sub>	X <sub>40</sub>	X <sub>62</sub>	X <sub>1012</sub>	X <sub>40</sub>	X <sub>62</sub>
67.0	.109	.643	.248	.020	.963	.017	.048	.001	.951
66.0	.160	.601	.239	.046	.933	.021	.077	.002	.921

```
T-Y-X (MMHG,C) 1012,40,62=760
67.,.109,.643,.020,.963,.048,.001,
66.,.160,.601,.046,.933,.077,.002
```

## ChemTran Pure Component Command Details

### ChemTran: Input Commands for Single Components

The correlations in DESIGN II for

- **K-values**
- **Enthalpies**
- **Densities**

of mixtures require basic information about the individual compounds in the mixture. For example, equations of state usually require the critical temperature, critical pressure, and/or the acentric factor for each chemical; activity coefficient correlations must be combined with pure component vapor pressures and equations of state to produce K-values; enthalpy calculations require ideal gas heat capacities.

**NOTE:** All of the above information is provided automatically for chemicals in the *Component Database Sorted By ID*

When a chemical is not in the Database ChemTran can predict and correlate all of the necessary data for use in DESIGN II.

This section describes commands to enter, regress, and predict pure component physical and thermodynamic properties. These commands and their corresponding options are summarized below. Next a Guidelines section containing detailed instructions and examples for all commands is presented in alphabetical order by group.

CONVENTIONS for commands and options in the following tables:

```
option 1
identifier(units option 2) i = data list
```

	option n
where	
identifier	is an abbreviation identifying a property. The required letters are bolded.
units	identifies the input units e.g., F for Fahrenheit, CM3/GMOL for cubic centimeters per gram-mole.
options	available for a particular command. Only one in a stack may be selected.. The top option in a stack is the default if none is selected.
i	is the component ID number
data list	is the list of data that is input by the user.

The following COMMAND is REQUIRED in ALL ChemTran input files:

**COM**ponents = i, j, k, .....

where i, j, k, ..... are the component ID numbers of the chemicals.

IF NO DATA is available for a chemical, then the ONLY other REQUIRED command for that chemical is:

**STRU**cture i =

This command is used to enter the bonding structure for nonstandard components. This structure information is used by ChemTran to calculate the molecular weight and estimate all the pure component properties required for DESIGN II. These estimates will be based on a hierarchy of techniques discussed in *ChemTran: Pure Component Property Generation*. If data has been entered for a specific property, then it will be used and the estimate bypassed. The hierarchy of estimation techniques can be overridden by inserting the appropriate property commands:

TB,TC,PC,VC or CP-T

See the individual command for details.

**Example 1.** Enter the bond data for isopropyl-tertbutyl ether. The structure can be Coded as:

**STRU**cture 200 = C1-C2,C3-C2,O4-C2,O4-C6,C6-C8,C7-C6,C5-C6

IF DATA IS available for a chemical, **THEN** the remaining commands fall into five groups:

1. Required Commands--**IF NO STRU** command is entered **OR IF** specific prediction techniques are desired.
2. Supplementary Commands--if not entered, the corresponding properties will be generated from commands in group 1.
3. K-value Commands--Used to enter tabular data for a single component. The data entered will override all K-value correlations in DESIGN II for the component.
4. Enthalpy Commands--Used to enter tabular data. When used tabular data must be entered for all components.
5. Table & Graph Commands--Used to print tables and graphs of pure component and binary data.

## Table 2.1 Single Component Commands

### Required Commands

**COM**ponents = i,j,k ..

**AMB** (units) i = (for petroleum fractions only),

**API** i = (for petroleum fractions only)

**NAME** i = up to sixteen characters

**MOL**ecular weight i =...

**DATA**

**OGA**t

**TB** (units, **STI**el) i =

**LYD**ersen forman thodos

**DATA**

**TC** (units, **LYD**ersen) i =

**FOR**man thodos

**DATA**

**PC** (units, **LYD**ersen) i =

**FOR**man thodos

**DATA**

**VC** (units, **LYD**ersen) i =

**YEN** Woods

**DATA** T\*\*2

**CP-T**(units,**CON**,T\*\*3) i =

**PAR**

**BEN**son

### Supplementary Commands

## Chapter 16

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**DATA**  
**VAP** or pressure  
**AC**entric factor ( **EDM**ister) i =  
**PEN**g Robinson  
**SOA**ve  
**APISOA**VE

**AMW** i = (for petroleum fractions only)

**DATA** **L**  
**L-T** (units, **CON**stants, **L\*\*1/2**) i =

**PAR**achore i =  
**ASS**ociation **PAR**ameter i =  
**DIP**ole **MOM**ent i =

**DATA**  
**CON**stants **LOGP**  
**P-T** (units, **THEK**, **LNPR**) i =  
**LNPR**, **LNP**

**DATA**  
**SUR**face **TEN**sion -**T** (units, **CON**stants) i =

**DATA**  
**V-T** (units, **CON**stants) i =  
**DATA**

**VS-T** (units, **CON**stants) i =  
**KMODPEN** (options) i =  
**SOL**ubility parameter i =

### K-Value Commands

**DATA** **K/T\*\*1/3**  
**K-T**(units, **CON**stants, **LNK** ) i =  
**INT**erpolative **LNKP**

### Enthalpy Commands

**DATA** **HL**  
**HL-T** (units, **CON**stants, **HL\*\*1/2**) i =,

**DATA** **HV**  
**HV-T** (units, **CON**stants, **HV\*\*1/2**) i =,

**DATA** **HS**  
**HS-T**(units, **CON**stants, **HS\*\*1/2**) i =,

### Transport Property Commands

**DATA**  
**THE CONL-T** (units, **CON**stants) i =  
**ROB**ins-Kingrea  
**SAT**o-Reidel  
**NBS81**

**DATA**  
**THE CONV-T** (units, **CON**stants) i =  
**ROY**-Thodos  
**EUC**ken  
**MOD**ified **EUC**ken

**DATA**  
**VISL-T** (units, **CON**stants) i =  
**ORR**ick-Erbar  
**NBS81**

**DATA**  
**VISV-T** (units, **CON**stants) i =  
**THO**dos  
**GOL**ubev

**DATA** **L**  
**L-T** (units, **CON**stants, **L\*\*1/2**) i =

### Table and Output Commands

**PRInt PROperties**

**LIQuid**  
**TABLE THE CON-T** (units, **VAPor**) i =

**LIQuid**  
**TABLE VIS-T** (units, **VAPor**) i =

**TABLE SURface-TENsion** (units) i =

**TABLE CP-T**(units) i =

**TABLE L-T** (units) i =

**TABLE P-T** (units) i =

**TABLE V-T** (units) i =

Abbreviations

<b>Cp</b>	Ideal Gas Heat Capacity
<b>L</b>	Latent Heat
<b>P</b>	Vapor Pressure
<b>SUR TEN</b>	Surface Tension
<b>V</b>	Volume

## ChemTran: Component Properties Command Details

The remainder of this section summarizes the options available for each identifier and corresponding data list requirements. Only the **UPPER CASE** letters indicated on a command are required. Lower case letters are used for explanation or to describe parameters that can be entered on the command. The various commands are listed in alphabetical order by groups.

Some methods of estimation require other data to be present. For example, the Lydersen method of estimating critical pressure requires that the molecular weight be available. Such requirements, if any, are shown with each command. For Data Base components, such "Other Data Required" is automatically available. For non-standard components, it must be entered on the commands indicated. Also, input commands can be used to override "Other Data Required" for data base components.

**ChemTran: Required Commands****ChemTran: Component Name**NAMing Components

**NAME** i =

Enter a name for your component. Maximum number of 16 characters no commas allowed. This command is used to label component i with a name of up to 16 characters. It is a required command for nonstandard components.

*Example:* **NAME** 200 = CHRYSENE

**ChemTran: COMponent Command**

**COM** = i,j,k,....

Enter the component ID number for those components listed in the Pure Component Database. The following component numbers are reserved:

<b>100 - 399</b>	Reserved for components not in the Pure Component Database. You <b>must</b> enter data for these components.
<b>100 - 199</b>	Reserved for Petroleum fractions
<b>200 - 299</b>	Reserved for Chemicals
<b>300 - 399</b>	Reserved for Solids.

For more details see:

**Component Database Sorted By ID**

Example 1. **COM**ponents = 1, 2, 3, 6, 100, 200 ID numbers correspond to the chemicals in the pure component database

1	Hydrogen
2	Methane
3	Ethane
4	Normal Butane

ID number 100 represents a petroleum fraction for which you must enter the AMB (average boiling point) and the API Gravity. ID number 200 represents a chemical which is not in the pure component database so you must enter physical property data.

**ChemTran: Critical Temperature**

**TC** (units,options) i = data list

## Chapter 16

This command is used to enter data directly or estimate the critical temperature of component i. The options are:

Options	Other Data Required	Data List	Comments
DATA+	none	Tc	enter Tc directly
LYDerson*	TB	none	Estimate Tc with Lydersen method
FORman*		none	
Thodos			

+default, assumed if no option entered

\*Requires STRUcture command to be entered for nonstandard components

**Example 1.** Enter the critical temperature for component 200 **TC** (C) 200 = 452,

**Example 2.** Use the Lydersen method to estimate Tc for component 200. Check for available molecular structures in *ChemTran Pure Component Property Generation*

**TC** (LYD) 200

### ChemTran: Critical Pressure

**PC** (units,options) i = data list

This command is used to enter data directly or estimate the critical pressure of component i, where i is the component ID number. The options are:

Options	Other Data Required	Data List	Comments
DATA+	none	Pc	enter Pc directly
LYDerson*	<b>MOL</b> ecular weight	none	estimate Pc with Lydersen method
FORman*		none	
Thodos			

+default, assumed if no option entered

\*Requires STRUcture command to be entered for nonstandard components

**Example 1.** Enter the critical pressure for component 200

**PC** (ATM) 200 = 2.0,

**Example 2.** Use the Lydersen method to estimate Pc for component 200. Check for available molecular structures in *ChemTran Pure Component Property Generation*. Requires a STRUcture command for component 200. See *ChemTran: Unified Group Contribution Technique* for use of the STRUcture command **PC** (LYD) 200

### ChemTran: Critical Volume

**VC** (units,options) i = data list

This command is used to enter data directly or estimate the critical pressure of component i, where i is the component ID number.

The options are:

Options	Other Data Required	Data List	Comments
DATA+	none	Vc	enter Vc directly
LYDerson*	none	none	estimate Vc by Lydersen method
YEN-Woods	<b>TB,TC,P</b>	none	best estimate obtained if liquid density supplied by <b>V-T</b> command

+default, assumed if no option entered

\*Requires STRUcture command to be entered for nonstandard components

**Example 1.** Enter the critical volume for component 200

**VC** (FT<sup>3</sup>/LBMOL) 200 = 174.2

**Example 2.** Use the Lydersen method to estimate Tc,Pc, Vc for component 205.

**VC** (LYD) 205

**TC** (LYD) 205

**PC** (LYD) 205

### ChemTran: Ideal Gas Heat Capacities

**CP-T** (units,options) i = TLL,TUL,data list

Using this command and the keywords for option1 and option2, the user may enter data for curve fitting, enter constants, or specify and estimation technique for the IDEaL gas heat capacity of component i. The option parameters are defined in the following tables. No other commands are required.

Option1	Option2	Data List	Comments
DATA+	T**2+	TLL,TUL ,Cp(T1),T1,,	enter data for curve fitting



	or T**3	Cp(T2),T2 up to 50 pairs	
<b>CON</b> stants	T**2+ T**3	TLL,TUL,	Enter 3 or 4 constants C1,C2,C3,C4 constants per option2
	SINH	TLL, TUL	C1, C2, C3, C4, & C5 constants per option2
<b>PAR</b> r*	T**2	none	Estimate by Parr method
<b>BEN</b> son*	T**3	none	Estimate by Benson method
Option2	Equation		
<b>T**2</b>	Cp = C1 + C2*T + C3*T2		
<b>T**3</b>	Cp = C1 + C2*T + C3*T2+ C4*T3		
<b>SINH</b>	Cp = C1 + C2 * {(C3/T)/Sinh(C3/T)**2 + C4*(C5/T)/Cosh(C5/T)**2 where C1, C2, C4 have CP units and C3, C5 have Temperature Units		

+default, assumed if no option is entered.

\*Requires the **STRU**cture command be entered for nonstandard components.

**NOTE:** Units for ideal gas heat capacity are entered in the following form: (CAL/GMOL/K,K)

A temperature parameter must be included in the unit description. The default unit option is: (BTU/LBMOL/R,F)

**Example 1.** Enter ideal gas heat capacity constants for component 205.

Coding: **CP-T** (CON,T\*\*3) 205 = 0.0,800.0,1.035062, .1815552, -.951961E-04, .1819259E-07,

**Example 2.** Specify the Benson Method for estimating the ideal gas heat capacity for component 200. Assume the **STRU**cture command has been entered for component 200.

Coding: **CP-T** (BEN) 200

### ChemTran: Molecular Weight

**MOL**eular weight i = data list

The molecular weight of component i is entered with this command. i is the component ID number. It is required for pure component data processing of nonstandard components. This command is not needed if the **STRU**cture command is used. The default molecular weight used for a solid (if none is entered) is 123.0 pounds per pound-mole.

*Example:* **MOL** 200 = 228.30

### ChemTran: Normal Boiling Point

**TB** (units,options) i = data list

This command is used to enter data directly or specify an estimation method for the normal boiling point of component i, where i is the component ID number.

Options may be specified as follows:

Option	Other Data-Required	Data List	Comments
<b>DAT</b> a+	none	Tb	enter Tb directly
<b>OGA</b> ta*	none	none	structure code estimate
<b>STI</b> el*	none	none	structure code estimate
<b>LYD</b> erson- Forman-Thodos	none	none	<b>STRU</b> cture command

+default, assumed if no option is entered

\*Requires **STRU**cture command for non standard components.

**Example 1.** Enter the boiling point for component 200.

**TB** (C,DAT) 200 = 448.0,

**Example 2.** Use the Stiel-Thodos estimation technique to determine the boiling point for component 200. Assume **STRU**cture command has been entered for component 200.

**TB**(STIel) 200

### ChemTran: Petroleum Fraction Commands

#### Average Boiling Point

**AMB** (units) i =

Enter the average boiling point for any component numbered 100-199 and 500-999. This command is to be used only for petroleum fractions.

## Chapter 16

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### API Gravity

API  $i$  =

Enter the API gravity for any component numbered 100-199 and 500-999. This command is to be used only for petroleum fractions.

**NOTE:** Default units for API Gravity is SPECIFIC GRAVITY not API

### Average Molecular Weight (Optional)

AMW  $i$  =

Enter the molecular weight for any component numbered 100-199 and 500-999. This command is to be used for petroleum fractions only. This is an optional command. If this command is not entered, ChemTran will generate a molecular weight using the values you entered for the required commands AMB and API.

### ChemTran: Supplementary Commands

#### ChemTran: Acentric Factor

ACentric factor (option)  $i$  = data list

This command provides these options for the acentric factor; The user may enter data, or request that ChemTran calculate it, or request that ChemTran estimate it. Since it is not a required command, if absent, ChemTran calculates the acentric factor from the vapor pressure, the critical pressure and critical temperature using the basic definition of the acentric factor by Pitzer.

Options	Other Data Required	Data List	Comments
DATA+	none	acentric factor	enter acentric factor directly
VAP	P-T	blank	acentric factor calculated from vapor pressure data
EDMister	TB,TC,PC	blank	estimate acentric factor with Edmister correlation.
PENg	TC,PC,P-T	blank	fit vapor pressure to Peng-Robinson equation.
SOAVE	TC,PC,P-T	blank	fit vapor pressure to SOAVE equation
APISOAVE	TC,PC,P-T	blank	fit vapor pressure to API version of the SOAVE equation

**NOTE:** +default - if no option is chosen ChemTran assumes that a data list has been entered.

**Example 1.** Have acentric factor calculated from user entered vapor pressure of component 200. Coding: ACE 200

**Example 2.** Use Edmister correlation to calculate the acentric factor for component 200 with data user has entered.  
Coding: ACE (EDM) 200

**Example 3.** Enter a value of .3 for the acentric factor for component 200. Coding: ACE 200 = .3

#### ChemTran: Acentric Factor

ChemTran offers five options for calculating the acentric factor. The default option does not require a direct input statement from the user. The other options are Edmister, Peng-Robinson, APISOAVE and SOAVE techniques. All require data for other physical properties to be present.

#### ChemTran: Default Acentric Factor Option

If vapor pressure data or correlations have been defined by the user, ChemTran automatically calculates the acentric factor using the definition,

$$\omega_i = -\log P_r (T_r = .7) - 1$$

where  $P_c$  and  $T_c$  are critical pressure and temperature, respectively.  $T_b$  is the normal boiling point and  $i$  is the component ID number.

**NOTE:**  $T_c$  and  $P_c$  commands are required for non-Data Base components.

**Example 1.** Use the default acentric factor estimation technique for component 200.

ACE 200 =  
PC (ATM) 200 = 27.3  
TC (C) 200 = 368

#### ChemTran: Edmister Acentric Factor Option

As an alternative to the default option, the user may specify the Edmister option for the acentric factor technique. This calculation requires data for  $T_c$ ,  $P_c$  and  $T_b$ .

$$\omega_i = 3/7 \left\{ \frac{T_b}{T_c - T_b} \right\} \log P_c \text{ where } P_c \text{ is in atmospheres.}$$

### Errors

This method should be used primarily as a check for other methods. In some cases it may provide results comparable to those obtained when estimated vapor pressure data is used with the default option. A small sampling of compounds (37) indicates for most straight chain (4 to 5 or less) hydrocarbons, alcohols and ketones, relative error will be around 5% or less. For branched hydrocarbons, the relative errors may be in the range of 10% or less.

**Example 1.** Use the Edmister technique to estimate the acentric factor for component 201 (201 is the component ID number).

Coding:

```
ACE (EDM) 201
PC (LYD) 201
TC (LYD) 201
TB 201 = 219.2
```

### ChemTran: PENg-Robinson Option for Acentric Factor

The user may also request calculation of an acentric factor resulting from fitting vapor pressure data to the Peng-Robinson equation.

**NOTE:** For non-standard components, TC, PC, TB and P-T commands are also required.

**Example 1.** Estimate an acentric factor by fitting vapor pressure data for component 200 to the Peng-Robinson equation.

Coding:

```
ACE (PEN) 200
PC 200 = 710.4
TC 200 = 552.22
P-T(C,MMHG) 200 = 60, 100, 450, 64, 6 50, 75.4, 760.4,
                  760, 80.14, 1000, 89.2
TB (C) 200 = 80.14
```

### ChemTran: SOAVE Option for Acentric Factor

The user may request calculation of an acentric factor by fitting vapor pressure data to the SOAVE equation of state.

**NOTE:** for non-standard components, entries for TC, PC, TB and P-T are also required.

**Example 1.** Use vapor pressure data from the Data Base to generate acentric factor for the SOAVE equation of state for CO<sub>2</sub>, H<sub>2</sub>S, methane and ethane (component ID numbers 49, 50, 2 and 3, respectively).

Coding:

```
ACE (SOAVE) 49
ACE (SOAVE) 50
ACE (SOAVE) 2
ACE (SOAVE) 3
```

### ChemTran: APISOAVE Option for Acentric Factor

The user may also supply a data input requesting calculation of the acentric factor by fitting vapor pressure data to the APISOAVE modified SOAVE equation of state. For non-standard components, entries for TC, PC, TB and P-T commands are also required.

**NOTE:** the acentric factors should not be recalculated for components for which interaction parameters are available in the APISOAVE technique. See *ChemTran: Table 1. APISOAVEK Interaction Parameter List* for the table of binary pairs contained in this technique.

**Example 1.** Use vapor pressure data from the Data Base to generate acentric factors for the API modification of the SOAVE equation for ethane and ethylene (component ID numbers 3 and 22, respectively). VLE data will be fitted to the APISOAVE equation.

Coding:

```
ACE (APISOAVE) 3
ACE (APISOAVE) 22
P-Y-X (C,ATM) 22, 3 = -17.8, 16.1, .15, .1, 17.4, 12837,.2, 20.8, .6, .5,
APISOAVEK
COM = 3,22
```

### ChemTran: Density Commands

Densities are entered using VOLume commands (V-T, VS-T). The units you specify determine whether values are densities or volumes.

### ChemTran: Liquid Volume

#### Liquid Volume (Density) Versus Temperature

V-T (units,options) i = TLL,TUL, data list

This command is used to provide ChemTran with either volume-temperature data for curve fitting or the appropriate constants for an equation  $V=f(T)$ . If the units are given as density units the program will assume that density data is in the data list.

**NOTE:** Units are required. Constants can only be entered for the volume equation

TLL = lower temperature limit of the data.

TUL = upper temperature limit of the data.

The options are:

## Chapter 16

Option	Required	Data List	Comments
DATA+	none	TLL,TUL,V(T1), T1,V1(T2),T2,	enter data for curve fitting up to 50 data pairs
CONstants	none	TLL,TUL,C1,C2,C3	enter constants for volume equation

+default, assumed if no option is entered

Volume data are fitted to the equation:  $V(T) = C1 + C2*T + C3*T^2$

Liquid volumes for pure components are used in calculations of activity coefficients for non-ideal solutions for the Wilson equation.

**Example 1.** Curve fit the following liquid density data for component 200.

V,lb/ft <sup>3</sup>	T,F	TLL	TUL
55.9	32.0	25	200
55.0	80.0		
53.6	130.0		
52.6	180.0		
51.4	190.0		

Coding: **V-T** (LB/FT<sup>3</sup>,F) 200 = 25,200,55.9,32,55.0,80,53.6,130,52.6,180,51.4,190

### ChemTran: Solid Volume

#### Solid Volume (Density) Versus Temperature

**VS-T** (units,options) i = TLL,TUL, data list

This command is used to enter volume-temperature data for curve fitting or volume constants for an equation  $V = f(T)$  for solid components. If the units are given as density units the program will assume that density data is in the data list.

**NOTE:** Units are required. Constants can only be entered for volume.

TLL = lower temperature limit for data  
TUL = upper temperature limit for data

The options are:

Option	Other Data Required	Data List	Comments
DATA+	none	TLL,TUL,Vs(T1),T1, Vs(T2),T2,...	Enter data for curve fitting up to 50 data pairs
CONstants	none	TLL,TUL,C1,C2,C3	Enter constants for volume equation*

+default, assumed if no option is entered

\*Volume data are fitted to the equation:  $Vs(T) = C1 + C2*T + C3*T^2$

**Example 1.** Curve fit the following solid density data for component 300:

V,FT <sup>3</sup> /LBMOL	T,F
0.12	32.0
0.18	100.0
0.22	500.0

Coding: **vs-T** (FT<sup>3</sup>/LBMOL,F) 200 = 0,1000,0.12,32,0.18,100,0.22,500

### ChemTran: Enthalpy of Liquid

**HL-T** (units,options) i = TLL,TUL,data list

This command allows the user to enter liquid enthalpy versus temperature data for data reduction to one of two equations. Alternatively, the command can be used to enter the constants for the equation directly. The parameters and options are:

Parameters: TLL = lower temperature limit where data is reliable  
TUL = upper temperature limit where data is reliable.

Option1	Other Data Required	Data List	Comments
DATA+	none	H1(T1),T1, H2(T2),T2,....	reduces data to equation given by option2 up to 50 pairs
CONstants	none	C1,C2,C3,	Constants for equation specified by option2

Option2	Equation
HL+	$H1 = C1 + C2*T + C3*T^2$
HL**1/2	$(H1)^{1/2} = C1 + C2*T + C3*T^2$

+default, assumed if no option is entered

**Example 1.** Enter liquid enthalpy data for component 202 and use the first equation option. The data is

H1(T),BTU/LB	T,F	TLL	TUL
139.2	0.0	0.F	300.F
169.0	50.0		
346.6	100.0		
392.9	200.0		
445.2	300.0		

Coding:

HL-T (BTU/LB,F,HL) 202 = 0.,300.,139.2,0.,169.0,50.,346.6,100.,392.9,200.,445.2,300.,

### ChemTran: Enthalpy of Solid

HS-T (units,options) i = TLL,TUL,data list

Solid enthalpy versus temperature data for data reduction by one of two equations are entered with this command. Alternatively, the command can be used to enter the constants directly. The parameters are:

Parameters: TLL = lower temperature limit where data is reliable  
TUL = upper temperature limit where data is reliable

Option1	Other Data Required	Data List	Comments
DATa+	none	Hs(T1),T1.... Hs(T2),T2,.....	reduces data to equation up to 50 pairs given by option2
CONstants	none	C1,C2,C3	Constants for equation specified by option2
Option2	Equation		
HS+	$H_s = C_1 + C_2 \cdot T + C_3 \cdot T^2$		
HS**1/2	$(H_s)^{1/2} = C_1 + C_2 \cdot T + C_3 \cdot T^2$		

+default, assumed if no option is entered

**Example 1.** Enter the following solid enthalpy data for compound 300. Use the second equation option.

Hs(T),BTU/LB	T,F	TLL	TUL
750	500	100F	1000F
785	520		
950	600		

Coding: HS-T (BTU/LB,F,DAT,HS\*\*1/2) 300 = 100,1000,750,500,950,600

### ChemTran: Enthalpy of Vapor

HV-T (units,options) i = TLL,TUL,data list

Vapor enthalpy versus temperature data for data reduction by one of two equations are entered with this command. Alternatively, the command can be used to enter the constants directly. The parameters are:

TLL = lower temperature limit where data is reliable

TUL = upper temperature limit where data is reliable

Option1	Other Data Required	Data List	Comments
DATa+	none	Hv(T1),T1, Hv(T2),T2,....	reduces data to equation up to 50 pairs specified by option2
CONstants	none	C1,C2,C3	Constants for equation specified by option2
Option2	Equation		
HV+	$H_v = C_1 + C_2 \cdot T + C_3 \cdot T^2$		
HV**1/2	$(H_v)^{1/2} = C_1 + C_2 \cdot T + C_3 \cdot T^2$		

+default, assumed if no option is entered

**Example 1.** Enter the following vapor enthalpy data for compound 200. Use the first equation option.

Hv(T),BTU/LB	T,F	TLL	TUL
445.2	300.0	300.F	500.F
473.0	350.0		
502.2	400.0		
532.9	450.0		
564.2	500.0		

Coding:

HV-T (BTU/LB,F,DAT,HV) 200 = 300.,500.,445.2,300,473.,350.,502.2,400.,532.9,450.,564.2,500.

### ChemTran: Kappa Parameter

#### Kappa Parameters for Modified Peng-Robinson

KMODPEN (option) i =

## Chapter 16

This command is used when specifying the modified Peng-Robinson equation of state and is required to specify the Kappa parameters. If the KMODPEN command is omitted, the kappa parameters will default to the form of the standards Peng-Robinson equation.

Kappa parameters are:

Option	Data List	Comments
<b>DATA</b>	K0,K1,K2,K3	Enter Kappa parameters
<b>VAP</b>	none	Kappa parameters are fitted to the P-T data entered by the user for nonstandard components, or the vapor pressure curve from DESIGN II's library for standard components.

### ChemTran: K-Value

#### K-value Versus Temperature

**K-T** (units,options) i = limits, data list

This command permits the user to enter K-values in the form of data, either for interpolation or curve fitting, or constants for one of three equation options. These equations give a functional dependence of K on T or K\*P on T. Any option2 parameter (the equation option) can be used with any option1 parameter.

Option1	Data List	Comments
<b>DATA+</b>	F(T1),T1,F(T2), T2,..... up to 50 F,T pairs	enter K-value data; F=K or K*P depending on option2; limits = TLL,TUL
<b>CON</b> stants	C1,C2,C3	enter constants for K-value equations; limits = TLL,TUL
<b>INT</b> erpolation	F(T1),T1,F(T2), T2,... up to 20 F,T pairs	enter K-value data for interpolation; F=K or K*P depending on option2; limits= TLL,TUL,PLL,PUL

#### Option2                      Equation

<b>K/T**1/3</b>	$(K/T)^{1/3} = C1 + C2*T + C3*T^2 + C4*T^3$
<b>LNK</b>	$\ln K = C1 + C2*T + C3/T^2$
<b>LNKP</b>	$\ln KP = C1 + C2*T + C3/T^2$

+default, assumed if no option is entered in the command line.

TLL = Lower temperature limit for data

TUL = Upper temperature limit for data

PLL = Lower pressure limit for data

PUL = Upper pressure limit for data

Any K-value data entered with the K-T command overrides ChemTran or DESIGN II internal data systems. When the INT option is used the program will automatically select data for the appropriate temperature and pressure range for interpolation. If the ranges are not valid then an internal data correlation system is used. Linear interpolation is performed on data for an equation of the form  $\ln K = f(1/T)$ .

**Example 1.** Enter K-value data for component 4. Use the LNK equation option.

Coding: K-T (R,LNK) 4 =  
310.,460.,1.26,360.,1.36,390.,1.57,410.,1.72,440.,

**Example 2.** Enter the same K-value data with pressure included (10 PSIA). Use the third equation option.

Coding: K-T (R,LNKP) 4 =  
310.,460.,12.6,360.,13.6,390.,15.7,410.,17.2,440.,

In examples 1 and 2 the data used is:

K	ToR
1.26	360.0
1.36	390.0
1.57	410.0
1.72	440.0

at a pressure of 10 PSIA and with temperature limits of 310R and 460R.

### ChemTran: Latent Heat

#### Latent Heat Versus Temperature

**L-T** (units,options) i = TLL,TUL,L1,T1,L2,T2,.... datalist

This command is used to enter latent heat data (heat of vaporization) for curve fitting or constants for one of two equations. Latent heat data is used for calculating enthalpy of a liquid. The parameters are:

TLL = lower temperature limit for data  
 TUL = upper temperature limit for data

<u>Option1</u>	<u>Other Data Required</u>	<u>Data List</u>	<u>Comments</u>
DATa+	none	L(T1),T1, L(T2),T2 up to 50 L,T values	enter data for curve fitting to equation specified by option2. If only one data point is entered the Watson method will be used to predict the latent Heat.
CONstants	none	C1,C2,C3	enter constants for latent heat equations

<u>Option2</u>	<u>Equation</u>
L+	$L = C1 + C2*T + C3*T^2$
L**1/2	$L^{**1/2} = C1 + C2*T + C3*T^2$

+default, this option is assumed if the command is entered without an option.

**Example 1.** Enter the following latent heat data for component 205. The data is reasonable over a temperature range 10 F to 230 F. Use the first equation option.

<u>L (BTU/LB)</u>	<u>T F</u>
456.7	100.0
443.6	155.0
424.4	196.0

Coding: **L-T** (BTU/LB,DAT) 205 = 10.,230.,456.7,100.,443.6,155.,424.4,196.,

### Notes on Latent Heat

If data **IS** regressed the C1, C2, and C3 constants would fit the equation:

$$L = C1 + C2*T + C3*T^2$$

If data **IS NOT** regressed the latent heat for water will be calculated by the equation:

$$L = 18.02*(75.0573 - 4260.42*(1 - Tr)^{1/3} + 3798.8*(1 - Tr)^{2/3} + 1595.99*(1 - Tr)^{4/3})$$

For substances other than water, IF **NO** data is regressed, the latent heat is calculated by the equation:

$$L = [C1*(1 - Tr)/(1 - C2/Tc)]^{0.38}; C3 = 1.0$$

If **NO DATA** is regressed the constants have the following meaning:

C1 = latent heat at the normal boiling point calculated by one of the above equations.

C2 = Normal boiling point in absolute temperature units.

C3 = 1.0 (not used)

### Liquid Heat Capacity Versus Temperature

**CPL-T** (units,options) i = TLL,TUL,CPL1,T1,CPL2,T2,.... datalist

This command is used to enter liquid heat capacity data for curve fitting or constants for one of two equations. Using this command and the keywords for option1 and option2, the user may enter data for curve fitting, or enter constants. Liquid heat capacity data is used for calculating enthalpy of a liquid. The option parameters are defined in the following tables. No other commands are required.

<u>Option1</u>	<u>Option2</u>	<u>Data List</u>	<u>Comments</u>
DATa+	T**2+ or T**3	TLL,TUL,CPL(T1),T1,, CPL(T2),T2 up to 50 pairs	enter data for curve fitting
CONstants	T**2+	TLL,TUL,	Enter 3 constants
	T**3	TLL,TUL,	C1,C2,C3,C4 constants per option2

<u>Option2</u>	<u>Equation</u>
T**2	$C_{PL} = C1 + C2*T + C3*T^{**2}$
T**3	$C_{PL} = C1 + C2*T + C3*T^{**2} + C4*T^{**3}$

+ default assumed, if no option is entered.

TLL, TUL – Temperature Lower Limit and Temperature Upper Limit

## Chapter 16

**NOTE:** Units for liquid heat capacity are entered in the following form:  
(CAL/GMOL/K,K)

A temperature parameter must be included in the unit description.  
The default unit option is:

(BTU/LBMOL/R,F)

*Example 1.* Enter liquid heat capacity constants for component 205.

Coding: **CPL-T** (CON,T\*\*3) 205 = 0.0,800.0,1.035062,.1815552,  
-.951961E-04,.1819259E-07,

*Example 2.* Enter the following liquid heat capacity data for component 205. The data is reasonable over a temperature range -15 F to 550 F. Use the T\*\*3 equation option.

CPL (BTU/LB/F)	T F
.416	-15.0
.492	145.0
.682	550.0

Coding: **CPL-T** (BTU/LB/F, F, T\*\*3) 205 = -15.0, 550.0, .416, -15.0, .492, 145.0, .682, 550.0,

### ChemTran: Surface Tension

#### SURface TENSion Versus Temperature

**SUR TEN-T** (units, option) i = TLL,TUL,data list

This command is used to enter surface tension data for a saturated liquid. It can also be used to select estimation technique for the surface tension.

The options are:

Options	Data List	Comments
<b>DATA+</b>	TLL,TUL,	enter data s1,T1,s2,T2, for curve fitting up to 50 pairs
<b>CONstants</b>	C1,C2	enter constants for surface tension equation.
<b>BRO BIR</b>	blank	estimate the surface tension with the Brodk-Bird technique. Requires Tc,Pc,Tb.
<b>MAC SUG*</b>	blank	estimate the surface tension with the MacLeod-Sugden technique.

+default assumed if no option is entered.

\*Requires STRUcture command be entered for nonstandard components.

Pure component surface tension data will be fitted to the equation:  
 $ST = C1(1.0-Tr)C2$  where 'ST' is the surface tension and Tr is the reduced temperature.

*Example 1.* Estimate the surface tension of propanol using the MacLeod and Sugden technique.  
Coding: **SUR TEN-T** (MAC SUG) 1023

*Example 2.* Estimate the surface tension of component 200 using the MacLeod and Sugden technique.  
Coding: **SUR TEN-T** (MAC SUG) 200

This example requires that a **STRU**cture command also be included.

### ChemTran: PRInt PROperties

The following command will provide a table of pure component properties for all of the components present in the components list.

#### **PRI PRO**

The following properties will appear in the output table:

Point Properties	Point Properties	Temperature Dependent Properties
Acentric Factor	Latent Heat At TB	Vapor Pressure
Characteristic Volume	Liquid Density At Tb	Ideal Gas Heat Capacity
Critical Compressibility	Liquid Volume At Tb	Surface Tension
Critical Density	Molecular Weight	Liquid Viscosity
Critical Pressure	Normal Boiling Point	Liquid Thermal Conductivity
Critical Temperature	Solubility Parameter	Vapor Thermal Conductivity
Critical Volume		
Density Factor		
Vapor Pressure At .85*TC		
Vapor Pressure At TB		



Enthalpy Factor  
 Vapor Pressure At Tb  
 Ideal Gas Heat Capacity At 500 K

### ChemTran: TABLEs of Property Versus Temperatures

**TABLE X-T**(units) i = initial T, final T, number of degrees per increment

This command is used to specify which saturated liquid property versus temperature table you want printed, the initial and final temperatures for the table, and the number of degrees per increment. These commands can be used for any component which is being defined with the **STRU**cture command or for any **PURE COMPONENT DATA BASE** components for which the appropriate properties versus temperature data are being entered. If no entry is made on the right hand side of the equals sign, 20 values will be printed over the temperature range of the saturated liquid. The available property options, **X** in the above command are as follows:

Option	Definition
<b>CP</b>	ideal gas heat capacity
<b>L</b>	latent heat
<b>P</b>	vapor pressure
<b>SUR TEN</b>	surface tension
<b>V</b>	volume

One property versus temperature option may be entered per **TABLE** command.

### ChemTran: Thermal Conductivity of Liquid

#### Thermal Conductivity of Liquid Versus Temperature

**THE CONL-T**(units,options) i = TLL,TUL, data list

This command is used to enter data for liquid thermal conductivity. Data can be fitted to a curve, correlation coefficients can be entered, or predictive methods may be specified.

TLL = lower temperature limit for data

TUL= upper temperature limit for data

Option1	Other Data Required	Data List	Comments
<b>DATa+</b>	none	TCONL(T1),T1, TCONL(T2), T2, Up to 50, TCONL,T values	enter data for curve fitting*
<b>CON</b> stants	none	C1,C2,C3	enter correlation coefficients*
<b>ROB</b> ins-Kingrea	Tc	none	
<b>SAT</b> o-Riedel	Tc,Tb	none	
<b>NBS81</b>	Tc,Pc,Vc,MW	none	

+default, assumed if no option is entered

\*data fit to the following equation

$$\text{LOG}_{10} \text{ THE CONL}(T) = C1/T + C2 + C3*T + C4*T^2;$$

where T is in units of R or K

**NOTE:** In order to use in DESIGN II choose **LNA**verage Thermal Conductivity option under Basic Thermo

### ChemTran: Thermal Conductivity of Vapor

#### Thermal Conductivity of Vapor Versus Temperature

**THE CONV-T**(units,options) i = TLL,TUL, data list

This command is used to enter data for vapor thermal conductivity. Data can be fitted to a curve, correlation coefficients can be entered, or predictive methods may be specified.

TLL = lower temperature limit for data

TUL= upper temperature limit for data

Option1	Other Data Required	Data List	Comments
<b>DATa+</b>	none	TCONV(T1),T1, TCONV(T2),T2,... Up to 50, TCONV,T values	enter data for curve fitting*
<b>CON</b> stants	none	C1,C2,C3,C4	enter correlation coefficients*
<b>ROY</b> -Thodos	Tb,Tc,Pc	none	
<b>EUC</b> ken	Tb,Tc,Pc	none	
<b>MOD</b> ified <b>EUC</b> ken	Tc,Pc, Vc, MW	none	

+default, assumed if no option is entered

\*data fit to the following equation

$$\text{LOG}_{10} \text{ THE CONV}(T) = C1/T + C2 + C3*T + C4*T^2;$$

## Chapter 16

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where T is in units of R or K

### ChemTran: Viscosity of Liquid

#### Viscosity of Liquid Versus Temperature

**VISL-T**(units,options) i = TLL,TUL, data list

This command is used to enter data for liquid viscosity. Data can be fitted to a curve, correlation coefficients can be entered, or predictive methods may be specified.

TLL = lower temperature limit for data

TUL= upper temperature limit for data

Other Data			
Option1	Required	Data List	Comments
<b>DATa+</b>	none	VISL(T1),T1, VISL(T2),T2, Up to 50 VISL,T values	enter data for curve fitting*
<b>CON</b> stants	none	C1,C2,C3,C4	enter correlation coefficients*
<b>ORR</b> ick-Erbar	Tb,Tc,Pc,	Vc,Mw	none
<b>NBS81</b>	Tb,Tc.Pc,	Vc,MW	none

+default, assumed if no option is entered

\*data fit to the following equation

$$\text{LOG}_{10} \text{VISL}(T) = C1/T + C2 + C3*T + C4*T^2;$$

where T is in units of R or K

### ChemTran: Viscosity of Vapor

#### Viscosity of Vapor Versus Temperature

**VISV-T**(units,options) i = TLL,TUL, data list

This command is used to enter data for vapor viscosity. Data can be fitted to a curve, correlation coefficients can be entered, or predictive methods may be specified.

TLL = lower temperature limit for data

TUL= upper temperature limit for data

Other Data			
Option1	Required	Data List	Comments
<b>DATa+</b>	none	VISV(T1),T1, VISV(T2),T2, Up to 50 VISV,T values	enter data for curve fitting*
<b>CON</b> stants	none	C1,C2,C3,C4	enter correlation coefficients*
<b>THO</b> dos	Tc,Pc,Mw	none	
<b>GOL</b> ubev	Tc.Pc,MW	none	

+default, assumed if no option is entered

\*data fit to the following equation

$$\text{LOG}_{10} \text{VISV}(T) = C1/T + C2 + C3*T + C4*T^2;$$

where T is in units of R or K

### ChemTran: STRUcture Command

**STRU**cture i = bonding data (where i is the component ID number).

This command is used to enter the bonding structure for nonstandard components. This structure information is used by ChemTran to calculate the molecular weight and estimate all the pure component thermophysical properties required for

DESIGN II. These estimates will be based on estimation techniques reported in literature and are proprietary. If data has been entered for a specific property, then it will be used and the estimate bypassed. The estimation techniques can be overridden by inserting the appropriate property commands,

**TB, TC, PC, VC, or CP-T**

with the option in parenthesis. See the individual commands ChemTran: Component Properties Command Details.

The command requires knowledge of the structure of bonding in the molecule. Coding of a structure requires three steps:

- Write down the structural formula of the molecule;
- Number all non-hydrogen atoms (It is not necessary to include information for any of the hydrogen atoms);
- Enter the bonding using the above command

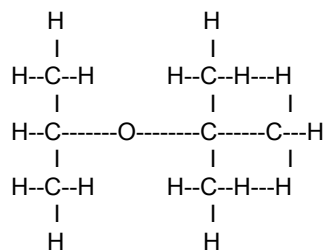
Symbols which are permitted for the structure are:

Bonds	
Type	Symbol
single bond	-
double bond	=
triple bond	*
Atomic Symbols	
Atom	Symbol
Boron	B
Bromine	BR
Carbon	C
Chlorine	CL
Fluorine	F
Hydrogen	H
Iodine	I
Nitrogen	N
Oxygen	O
Silicon	SI
Sulfur	S

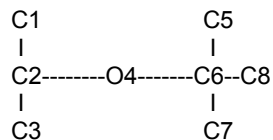
The bonding data required to describe the chemical structure is illustrated in several examples which follow. After ChemTran has processed the structure data and generated physical properties, a drawing of the structural formula will be provided as a check on the bonding information which was entered.

**Example 1.** Enter the bond data for isopropyl-tertbutyl ether.

The structure is:



which can be numbered as



ChemTran then automatically inserts hydrogen to meet valency requirements.

**Coding:**

**STRU 200** = C1-C2, C3-C2, O4-C2, O4-C6, C6-C8, C7-C6, C5-C6,

**ChemTran: Vapor Pressure**

**Vapor Pressure Versus Temperature**

## Chapter 16

P-T (units,options) i = TLL,TUL,P1,T1,P2,T2,...data list

This command is used to enter: Vapor pressure versus temperature data for curve fitting, or Constants for one of three vapor pressure equations. There are two options: Option 1 defines whether data entered are constants or data, and Option 2 specifies which of the four vapor pressure equations is to be used.

Option 1	Option 2	Other Data Required	Data List	Comments
DATA+	LOGP	none	TLL,TUL, P1,T1,	enter data for equation one up to 50 pairs
	LNP	none	-do-	enter data for equation two
	LNPR1	TB,TC,PC	-do-	enter data for equation three
	LNPR2	TB,TC,PC	-do-	enter data for equation four
CONstants	LOGP	none	TLL,TUL,	enter constants for equation one C1 thru C6
	LNP	none	TLL,TUL,	enter constants for equation two C1 thru C6
	LNPR1	TB,TC,PC	C2,C3	for IDs << 1000
	LNPR2	TB,TC,PC	C1,C2,C3,C4	for IDs >> 1000
	THEK	none	TB,L-T,TC,PC	Est. Pv(T) with Thek-Stiel correlation; requires data for Hv, Tc, Pc, Tb
LNPR	none	TB,TC,PC	blank	Estimates Pv(T) with LNPR correlation based on reduced Tc,Pc,

### Option 2 Equation

EQN 1: LOGP Vapor Pressure =  $10^{\{C_1 + C_2 / (C_3 + T) + C_4 * T + C_5 * T^2 + C_6 * \text{Log } T\}}$

EQN 2: LNP Vapor Pressure =  $\text{Exp}\{C_1 + C_2 / (C_3 + T) + C_4 * T + C_5 * T^2 + C_6 * \text{Ln } T\}$

EQN 3: LNPR1 Vapor Pressure =  $P_c * 10^{\{(-C_2 / T_r) * (1 - T_r^2 + C_3 * (3 + T_r) * (1 - T_r)^3)\}}$   
For Component ID # < 1000

EQN 4: LNPR2 Vapor Pressure =  $P_c * 10^{\{C_1 + C_2 / T + C_3 * T + C_4 * T^3\}}$   
For Component ID # >= 1000

Note: For all component ID's at  $P > P_{ci}$  (supercritical) and  $T_r > 1$

$$\text{Vapor Pressure} = P_c * 10^{\{C_5 * (T_r - 1) / T_r\}}$$

+default, assumed if no option is entered (see example 1)

\*Reid-Plank-Miller vapor pressure equation

NOTE: If you enter constants, be sure the equation to which your data was fitted matches one of the preceding equations. If it is of the form  $A - B / (C + T)$ , then adjust the sign of your second constant accordingly.

LNPR equation is represented in this section as  $\text{LOG } P = \dots$ . This is a base 10 logarithm not a natural log as the key word LNPR might imply.

Example 1. Enter the following vapor pressure data for curve fitting for component 201. Use the logP vapor pressure equation.

Pressure mm of Hg	Temperature T, C	Limit	
		Upper	Lower
10.0	-108.51	-25.4C	-108.51 C
40.0	-92.44		
100.0	-79.63		
700.0	-43.92		
1500.0	-25.4		

### Coding:

P-T (MMHG,C) 201 =108.51,-25.4,10.,-108.51,40.,-92.44,100.,-79.63,700.,43.92,1500,-25.4,

Units are shown but No option is selected so the default is logP for DATA.

## ChemTran: Vapor Phase Association Commands

### Association Parameter

ASSociation PARAmeter i =

Enter the association parameter for component i. This data is required for the Hayden O'Connell and Chemical theory vapor fugacity methods.

### Dipole Moment

DIPole MOMent i =

Enter the dipole moment for component i. This data is required for the Hayden O'Connell and Chemical theory vapor fugacity methods.

### Parachore

PAR i =

Enter the parachore for component i. This data is required for the Hayden O'Connell and Chemical theory vapor fugacity methods.

## ChemTran Pure Component Property Generation

Many methods for estimating pure component properties are available in ChemTran as user options. This section describes the techniques for predicting the following:

1. *ChemTran: Normal Boiling Point Estimation*
2. *ChemTran: Critical Property Methods* (critical temperature, pressure and volume)
3. *ChemTran: Ideal Gas Heat Capacity Methods*
4. *ChemTran: Vapor Pressure Methods*
5. *ChemTran: Acentric Factor Methods*
6. *ChemTran: Volume (Density) Methods*
7. *ChemTran: Characteristic Volume Method*
8. *ChemTran: Latent Heat Methods*
9. *ChemTran: Solubility Parameter Method*
10. *ChemTran: Surface Tension Methods*

Predictive techniques for the first three sets of properties consist of group contribution methods. The remainder of the properties are estimated from various data correlations and/or group contribution techniques.

### ChemTran: Normal Boiling Point Estimation

ChemTran includes two group contribution methods for predicting the normal boiling point of a non-standard component. Both of these methods require only a description of the component's molecular structure which is entered with the STRUcture command. These two methods are described below.

In addition to the method descriptions, a brief discussion of the errors associated with each method is included. Equally important, an outline of the range of applicability for chemical types is presented. It is very important to examine this material before selecting a predictive technique.

#### **ChemTran: Ogata and Tsuchida Method**

This is a relatively reliable method for a range of chemicals where it is applicable. Ogata and Tsuchida compared predicted values with experimental values for 600 compounds and found the following distribution of errors:

**Table 7.1**  
Error Distribution for  
Ogata - Tsuchida Estimate of  $T_b$

% of Compounds	Dev. From Experimental Boiling Points in °C
80	0° to 2° C
11	2° C to 3° C
7	3° C to 4° C
2	4° C to 5° C

The larger errors are generally incurred for the initial members (usually methyl and seldom ethyl) of a homologous series.

Tables 7.2 and 7.3 list the functional groups that are available to this method. If a component is comprised only of the functional groups in these tables its boiling point may be estimated with this method.

**Table 7.2**  
Functional Groups for  
Ogata-Tsuchida Estimate of  $T_b$

NOTE: Symbols are defined at end of table.

<b>RX</b>	<b>Groups, R, showing Deviation &gt; 5° K</b>
RH	Me, t-Bu
RCI	
RBr	
RI	
ROH	Me, t-Bu
MeOR	Me
EtOR	
ROR	Me, Hep
PhOR	
RONO <sub>2</sub>	
RSH	
RSM <sub>e</sub>	Me
RSEt	

# Chapter 16

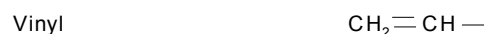
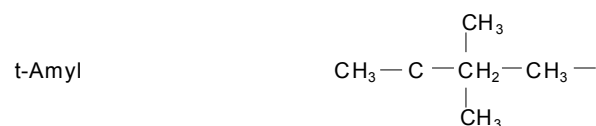
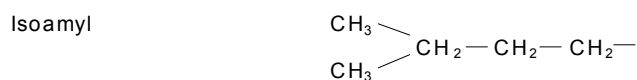
RSR	Me, Hep
RNH <sub>2</sub>	
RNHMe	
RNHet	
RNHPr	
RNMe <sub>2</sub>	Me
RNO <sub>2</sub>	Me, Et
HCOR	
MeCOR	
EtCOR	
RCN	
RCOCl	
HCOOR	
MeCOOR	
EtCOOR	
PhCOOR	
RCOOH	
RCOOMe	
RCOOEt	
RCOOPr	
RCOOPh	
(RCO) <sub>2</sub> O	Hep
ClCH <sub>2</sub> COOR	
ClCHCOOR	
BrCH <sub>2</sub> COOR	
NCCH <sub>2</sub> COOR	
CH <sub>2</sub> = CHCOOR	

t-Bu = tert - butyl group  
 Et = ethyl group  
 Hep = heptyl group  
 Me = methyl group  
 Ph = phenyl or benzyl group  
 Pr = propyl group  
 R = functional group in Table 7.3

**Table 7.3.**

Alkyl Groups for  
Ogata-Tsuchida Estimate of Tb

Methyl	CH <sub>3</sub> —
Ethyl	CH <sub>3</sub> — CH <sub>2</sub>
n-Propyl	CH <sub>3</sub> — CH <sub>2</sub> — CH <sub>2</sub>
Isopropyl	$\begin{array}{c} \text{CH}_3 \\ \diagdown \\ \text{CH}_2 \\ \diagup \\ \text{CH}_2 \end{array} \text{—}$
n-Butyl	CH <sub>3</sub> — CH <sub>2</sub> — CH <sub>2</sub> — C <sub>2</sub> —
sec-Butyl	$\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3 \text{—CH}_2 \text{—CH}_2 \text{—} \end{array}$
Isobutyl	$\begin{array}{c} \text{CH}_3 \\ \diagdown \\ \text{CH}_2 \\ \diagup \\ \text{CH}_3 \end{array} \text{—CH}_2 \text{—CH}_2 \text{—}$
t-Butyl	$\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3 \text{—C—} \\   \\ \text{CH}_3 \end{array}$
n-Amyl	CH <sub>3</sub> — CH <sub>2</sub> — CH <sub>2</sub> — CH <sub>2</sub> —



### ChemTran: Stiel and Thodos Method

This is a method for estimating the normal boiling points of saturated aliphatic hydrocarbons. The reliability of the method is very good for the range of compounds where it is applicable. An error analysis was performed by Stiel and Thodos and is illustrated in the following table.

**Table 7.4.**

Error Analysis for Stiel-Thodos Estimate of Tb

Type of Molecu.e	No. Tested	Average Deve. In °K	Percent Deviation
propane	1	0.23	0.10
butanes	2	0.25	0.24
pentanes	3	0.19	0.06
hexanes	5	0.19	0.06
heptanes	9	0.59	0.16
octanes	18	0.66	0.17
nonanes	35	1.30	0.33
decanes	75	2.87	0.66

To use this method, only the STRUcture command is necessary and ChemTran automatically calculate the following parameters necessary for this method.

1. the number of carbon atoms
2. for isomers; the polarity number, which is the total pairs of C atoms separated by three single C-C bonds
3. for isomers; the branch code - a series of numbers indicating the number of carbon atoms on either side (not both sides) of each C-C bond.

### ChemTran: Critical Property Methods

Several options are available in ChemTran for estimating the critical temperature  $T_c$ , critical pressure  $P_c$ , and critical volume  $V_c$  of a chemical. With one exception, they are all group contribution techniques. The exception is for  $V_c$  where one technique

## Chapter 16

is based on a correlation of critical properties and liquid densities. Any option is automatically invoked by specifying the keyword parameter on the appropriate input command. The following discussion provides descriptions, sample applications and examples of the input commands for each of these methods. All input commands for pure component properties are summarized in ChemTran: Input Commands For Single Components.

### **ChemTran: Lydersen Method for $T_c$ , $P_c$ , and $V_c$ Estimation**

The Lydersen Method is a group contribution technique for estimating  $T_c$ ,  $P_c$ , and  $V_c$ . The STRUcture command needs to be entered and ChemTran will automatically determine which of the Lydersen groups in Table 7.5 are present and calculate the estimated critical properties. However, for  $T_c$  and  $P_c$  some additional information is required; for  $T_c$  the normal boiling point and for  $P_c$  the molecular weight. These may be entered directly or estimated by the structure command.

This method is applicable to a wide range of compounds with good reliability. Error analyses for over 170 compounds are given in the following table.

**Table 7.5.**  
Error Analysis for  
Lydersen Group Method

Compound Type	Number Tested			%Deviation		
	$T_c$	$P_c$	$V_c$	$T_c$	$P_c$	$V_c$
hydrocarbons	60	60	60	0.7	2.9	2.2
alkylbenzenes	17	17	15	0.6	2.2	1.4
halogenated hydrocarbons (including halobenzenes)	27	22	15	0.8	5.3	2.9
Alcohols and ethers esters	19	11	8	1.8	3.5	1.8
acids	27	15	15	1.1	2.8	2.5
ketones	6	4	4	0.9	10.6	2.0
	2	2	2	0.1	0.7	4.4

As with all estimation methods, this table should serve as a guide for evaluation for errors.

**Table 7.6.**  
Functional Groups  
Available for the Lydersen Method

Bond Type	Bond Type	Bond Type	Bond Type
<b>Non-ring increments</b>	<b>Oxygen increments</b>	<b>Ring increments</b>	<b>Nitrogen increments</b>
— CH <sub>3</sub>	— OH (alcohols)	— CH <sub>2</sub> —	— NH <sub>2</sub>
— CH <sub>2</sub>	— OH (phenols)	— CH —	— NH (non-ring)
— CH	— O— (non-ring)	— C —	— NH (ring)
— C —	— O— (ring)	= CH	
		= C —	— N— (non-ring)
= CH <sub>2</sub>	C — O = (non-ring)	= C =	— N— (ring)
= CH	C — O = (ring)		



$\begin{array}{c}   \\ \text{=C-} \end{array}$	$\begin{array}{c}   \\ \text{HC=O} \end{array}$ (aldehyde)	<b>Halogen - Increments</b>	
$\text{=C=}$	$\text{-COOH}$ (acid)	$\text{-F}$	$\text{-NO}_2$
$\equiv\text{CH}$	$\text{-COO}$ (ester )	$\text{-Cl}$	
$\equiv\text{C-}$	$\text{=O}$ (except for combinations above)	$\text{-Br}$	
		$\text{-I}$	
		<b>Sulfur increments</b>	<b>Miscellaneous</b>
		$\text{-SH}$	$\text{-Si-}$
		$\text{-S-}$ (non-ring)	$\text{-B-}$
		$\text{=S}$	

### **ChemTran: Yen-Woods Estimate of Critical Volume**

This estimation technique is based on a temperature, pressure and critical compressibility correlation. Best results are obtained if the user supplies a liquid density; however, if liquid densities are not available ChemTran will default to an estimate based on the critical properties,  $T_c$  and  $P_c$ .

The basis of this method is a correlation of liquid densities for sixty-two compounds, chosen to represent a large variety of organic and inorganic chemicals. In a comparison between calculated and experimental data for 693 points the average error was 2.1%. A maximum deviation of 10% was observed for methylcyclohexane, but this difference was attributed to possible inaccuracies in experimental data for this compound.

The following considerations should be observed when using this technique:

1. The input file must contain an input command for  $T_c$ ,  $P_c$ , and  $T_b$ , if the component is not in Data Base.
2. Best results are obtained by specifying a liquid density using the V-T input command (see ChemTran: Liquid Volume (Density) for details)

**Example 3.** The input commands are

**VC (YEN) 62 =**

**V-T(CM3/G,C) 62 = 0.,50., 1.00,0.0**

These commands will produce an estimate of VC for water, component 62, based on database values of  $T_c$  and  $P_c$  and the input V-T data.

---

## **ChemTran: Ideal Gas Heat Capacity Methods**

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ChemTran contains two options for estimating the ideal gas heat capacities for a molecule. Both are group contribution techniques and are generally referred to as the Benson method and Parr method. The Benson method, as a general rule, will provide somewhat better results than the Parr method when it is applicable. Neither method requires any other data than the molecular structure which is entered with the STRUcture command.

### **ChemTran: Parr Estimation Technique**

This group contribution technique is relatively simple to use and is applicable to a very broad variety of organic compounds. From the molecular structure, ChemTran will calculate:

1. number of atoms,
2. number of freely rotating non H-atom bonds, and
3. the number and code specifications for each bond type.

The different bond types and their corresponding code numbers are listed in Table 7.7. For this method, the focus is on the type of bond rather than the substituent atom or group.

This bond data is used in the Parr method to estimate the coefficients a, b, and c in the following equation:

$$C_p \text{ } ^\circ(T) = a + bT + cT^2$$

Ideal gas heat capacities from this equation are considered valid for a temperature range of about 300° K to 1500° K.

### **Errors**

For most compounds, the Parr method predicts ideal gas heat capacities to within 10%. Errors may be expected to be smaller with straight chain hydrocarbons and increase with branching and degree of unsaturation. Predictions for halogenated compounds may be in error by 10%. The errors for other compounds have not been tabulated.

**Table 7.7.**

Bond Types Available to the Parr Method

### Bond Type

C-C≠  
C-C+  
C=C  
C=C  
C-H  
C-O  
C=O  
C-N  
C N  
C-Cl  
C-F  
C-Br  
C-I  
O-H  
S-H  
S=O  
C-S  
N-N^

≠ ALIPHATIC

+ Aromatic and conjugated double bonds

^ Not for N<sub>2</sub>O or N<sub>2</sub> O<sub>4</sub>

### References:

1. B.L. Crawford and R. G. Parr, J. Chem. Phys., 16:233 (1948)";
2. R. V. Meghreblian, J. Am. Rocket Soc., September, 1951, p.128."
3. "The Properties of Gases and Liquids", Reid and Sherwood (Second Edition)(Pages 178 and 254 of Chapter 5)

### ChemTran: Benson Estimation Technique

The Benson method provides a little more reliability for the estimation of ideal gas heat capacities. It offers a more accurate description of a larger variety of chemicals. The method used in ChemTran is based closely on that presented by Benson, et al., but has been modified to include a larger variety of chemicals. Additional data have also been used to determine some group contributions in order to improve the accuracy of the technique.

Enter the non-standard component's molecular structure with the ChemTran: STRUcture command and ChemTran will automatically determine which Benson groups are present and will estimate the ideal gas heat capacity.

### Errors

Instead of three coefficients, the Benson method estimates four coefficients for the following equation:

$$C_p^{\circ} (T) = a + bT + cT^2 + dT^3$$

As a consequence, the temperature dependence of  $C_p^{\circ}$  is represented more accurately than for the Parr method. Errors for hydrocarbons with moderate branching or unsaturation usually are less than 2% to 3%. For greater branching and degree of unsaturation, these errors are usually less than 4% to 5%. Although no detailed tabulation has been prepared for other chemicals, generally, an upper bound of 5% can be assigned to the error.

Tables 7.8 - 7.10 describe the functional groups available to the Benson Method.

**Table 7.8.**  
Available Benson Carbon Groups

<u>Type</u>	<u>Description</u>	<u>Symbol</u>
	Single bonded carbon atom	C
-C=	Double bonded carbon atom & terminal allenic carbon atom	Cd
-C≡	Triple bonded carbon atom	Ct
C	Aromatic carbon atom	Cb
	Allenic C atom, represents central atom only	Ca

**Table 7.9.**

Available N Benson Groups

<u>Type</u>	<u>Description</u>	<u>Symbol</u>
= N - H	double bonded in an imine	N <sub>i</sub>
- N = N-	double bonded in an azo compound	N <sub>a</sub>
	in a pyridine ring	N <sub>i</sub> -(C <sub>B</sub> )
All others	—	N

**Table 7.10.**

Available Hydrocarbon Benson Groups

<u>Bond Type</u>	<u>Bond Type</u>
C - (H)3 (C)	Cd - (Cd) (H)
C - (H)2 (C)2	Cd - (Cd) (C)
C - (H) (C)3	{ Cd - (Cd) (H) }
C - (C)4	Cd - (CB) (C)
Cd(H)2	{Cd - (Ct)(H)}
Cd - (H) (C)	C - (Cd) (C) (H)2
Cd - (C)2	C - (Cd)2 (H)2
C - (Cd)(C)(H)2	Ct - (C)
C - (Ct)(C)(H)2	Ct - (Cd)
C - (CB)(C)(H)2	CT - (CB)
C - (Cd)(C)2 (H)	CB - (H)
C - (Ct)(C)2 (H)	CB - (C)
C - (CB)(C)2 (H)	CB - (Cd)
C - (Cd)(C)3	{CB - (Ct)}
C - (CB)(C)3	CB - (CB)
Ct - (H)	Ca

**OXYGEN-CONTAINING GROUPS**

## Chapter 16

### Bond Type

CO - (O)(C<sub>d</sub>)  
 CO - (O)(C)  
 {CO - (O)(H)<sup>f</sup>}

CO (C)<sub>2</sub>

CO - (C)(H)  
 CO - (H)<sub>2</sub>  
 O - (CO)(C)  
 O - (CO)(H)<sup>g</sup>  
 O - (O)(O)<sup>f</sup>

O - (O)(C)

O - (O)(H)

{O - (C<sub>B</sub>)(H)<sup>g</sup>}

O (C)

O (C)(H)

{C<sub>d</sub> - (CO)(H)<sup>e</sup>}

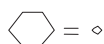
{C<sub>d</sub> - (O)(H)}

### Bond Type

CB - (O)  
 C - (CO) (C) (H)<sub>2</sub>  
 {C (CO)(H)<sub>3</sub><sup>a</sup>}

C - (O) (C<sub>d</sub>)(H)<sub>2</sub>

C - (O) (C)<sub>3</sub>  
 C - (O) (C)<sub>2</sub> (H)  
 C - (O) (C)(H)<sub>2</sub>  
 {C - (O) (H)<sub>3</sub><sup>h</sup>}



### NITROGEN-CONTAINING GROUPS

#### Bond Type

{C - (N)(H)<sub>3</sub><sup>j</sup>}

C - (N)(C)(H)<sub>2</sub>

C - (N)(C)<sub>2</sub>(H)

C - (N)(C)<sub>3</sub>

N - (C)(H)<sub>2</sub>

N - (C)<sub>2</sub> (H)<sub>2</sub>

N - (C)<sub>3</sub>

N - (N) (H)<sub>2</sub>

N - (N) (C)(H)

NI - (C<sub>B</sub>)

NA - (H)

N - (C<sub>B</sub>) (H)<sub>2</sub>

CB - (N)

#### Bond Type

CO - (N) (H)

CO - (N) (C)

N - (CO)(H)

C - C (CN) (C)(H)<sub>2</sub>

C - (CN)(C)<sub>2</sub> (H)

C<sub>d</sub> - (CN) (H)

C<sub>d</sub> - (NO<sub>2</sub>) (H)

C<sub>B</sub> - (CN)

C<sub>t</sub> - (CN)

C - (NO<sub>2</sub>) (C)(H)<sub>2</sub>

C - (NO<sub>2</sub>) (C)<sub>2</sub> (H)

O - (NO) (C)

O - (NO<sub>2</sub>) (C)

**HALOGEN-CONTAINING GROUPS**

<u>Bond Type</u>	<u>Bond Type</u>
Cd - (F) <sub>2</sub>	Cd - (Cl) (H)
Cd - (Cl) <sub>2</sub>	Cd - (Br) (H)
Cd - (Br) <sub>2</sub> (H)	Cd - (I)(H)
Cd - (F)(Cl)	Ct - (Cl)
Cd - (F)(Br)	Ct - (Br)
Cd - (Cl)(Br)C <sub>t</sub> - (I)	
Cd - (F)(H)	

**ARENES**

C <sub>B</sub> - (F)	C - (Cl)(H) <sub>2</sub> (C)
C <sub>B</sub> - (Cl)	C - (Cl) <sub>2</sub> (C) <sub>2</sub>
C <sub>B</sub> - (Br)	C - (Cl)(H) (C) <sub>2</sub>
C <sub>B</sub> - (I)	C - (Cl) (C) <sub>3</sub>
C - (C <sub>B</sub> ) (F) <sub>3</sub>	C - (Br) <sub>3</sub> (C)
C - (F) <sub>3</sub> (C)	C - (Br) (H) <sub>2</sub> (C)
C - (F) <sub>2</sub> (H) (C)	C - (Br) (H) (C) <sub>2</sub>
C - (F) (H) <sub>2</sub> (C)	C - (Br)(C) <sub>3</sub>
C - (F) <sub>2</sub> (C) <sub>2</sub>	C - (I) (H) <sub>2</sub> (C)
C - (F) (H) (C) <sub>2</sub>	C - (I) (H) (C) <sub>2</sub>
C - (F) <sub>2</sub> (Cl) (C)	C - (I) (C) <sub>3</sub>
C - (Cl) <sub>3</sub> (C)	C - (Cl) (Br) (H) (C)
C - (Cl) <sub>2</sub> (H) (C)	C - (Cl) (C) (O) (H)

**SULFUR-CONTAINING GROUPS**

<u>Bond Type</u>	<u>Bond Type</u>
{ C - (H) <sub>3</sub> (S) }	S - (S) (C)
C - (C) (H) <sub>2</sub> (S)	S - (S) <sub>2</sub>
C - (C) <sub>2</sub> (H) (S)	{ C - (SO) (H) <sub>3</sub> }
C - (C) <sub>3</sub> (S)	SO - (C) <sub>2</sub>
{ C <sub>B</sub> - (S) }	{ C - (SO)H <sub>3</sub> }
{ C <sub>d</sub> - (H) (S) }	SO <sub>2</sub> - (C) <sub>2</sub>
C <sub>d</sub> - (C) (S)	{ CO - (S) (C) }
C - (C) (H)	S - (H) (CO)
S - (C <sub>b</sub> ) (H)	S - (C) (CN)
S - (C) <sub>2</sub>	{ CS - (N) <sub>2</sub> }
S - (C <sub>d</sub> ) <sub>2</sub>	N - (CS) (H) <sub>2</sub>

**ChemTran: Vapor Pressure Methods**

Vapor pressure data may be estimated for a pure component in ChemTran by one of two methods. Both methods are based on correlations of data for a wide variety of compounds. Also, both methods require the user to enter commands for other property data into the ChemTran input file. For this data, the user has the choice of utilizing literature data or the estimation techniques furnished as options in ChemTran. These methods are used by ChemTran to calculate vapor pressures from the triple point to the critical temperature. A special default option is used if vapor pressures are required for supercritical conditions.

A straight line, joining the boiling point and critical point, is used to calculate vapor pressures above the critical.

**ChemTran: Thek-Stiel Correlation**

The Thek-Stiel correlation for vapor pressure is suitable for both polar and non-polar chemicals. It should be better than other correlations for polar and hydrogen-bonded substances at temperatures below the boiling point. However, it requires that  $T_b$ ,  $T_c$ , and  $\Delta H_v$  be supplied to ChemTran, either as data or by estimation techniques.

Thek and Stiel checked this method for 69 polar and non-polar chemicals. The average error was about 1% and the maximum error was usually less than 5%. The command for this method is:

**P-T (THEK) 200**

where 200 is the component ID number.

**NOTE:** TC, PC, TB and L-T commands must also be entered.

**ChemTran: LNPR Vapor Pressure Correlation**

This vapor pressure correlation is applicable for a variety of organic and inorganic compounds. It can be used for temperatures ranging from the triple point to the critical point. Since this is a reduced equation, values for  $T_c$ ,  $P_c$  and  $T_b$  are required.

## Chapter 16

A guide to the accuracy which can be expected from this method is given in the following table for three classes of compounds.

**Table 7.12.**  
Error Characteristics for LNPR Correlation

<b>Compound Type</b>	<b>No. of Compounds</b>	<b>% Mean Deviation</b>	<b>Range</b>
hydrocarbons	34	0.27	10-1500 mm
non-polar organics	45	0.48	10-1500 mm
polar organics	8	0.60	10-1500 mm
inorganics	18	0.34	10-1500 mm
mixtures, mostly inorganic	24	0.55	Tb to Tc

The user should also be aware that at low pressures the correlation may not be too good for liquids such as alcohols and carboxylic acids. This is true of other vapor pressure estimations also. Inaccuracies introduced at these conditions will vary for each case and will, therefore, need to be judged on an individual basis.

The command for this method is of the form

**TB** (units, options) i = data

**TC** (units, options) i = data

**PC** (units, options) i = data

---

### ChemTran: Acentric Factor Methods

---

ChemTran offers five options for calculating the acentric factor. The default option does not require a direct input statement from the user. The other options are Edmister, Peng-Robinson, APISOAVE and SOAVE techniques. All require data for other physical properties to be present.

#### ChemTran: Default Acentric Factor Option

If vapor pressure data or correlations have been defined by the user, ChemTran automatically calculates the acentric factor using the definition,

$$\omega_i = -\log P_r (T_r = .7) - 1$$

where  $P_c$  and  $T_c$  are critical pressure and temperature, respectively.  $T_b$  is the normal boiling point and  $i$  is the component ID number.

**NOTE:**  $T_c$  and  $P_c$  commands are required for non-Data Base components.

**Example 1.** Use the default acentric factor estimation technique for component 200.

```
ACE 200 =  
PC (ATM) 200 = 27.3  
TC (C) 200 = 368
```

#### ChemTran: Edmister Acentric Factor Option

As an alternative to the default option, the user may specify the Edmister option for the acentric factor technique. This calculation requires data for  $T_c$ ,  $P_c$  and  $T_b$ .

$$\omega_i = 3/7 \left\{ \frac{T_b}{T_c - T_b} \right\} \log P_c \text{ where } P_c \text{ is in atmospheres.}$$

#### **Errors**

This method should be used primarily as a check for other methods. In some cases it may provide results comparable to those obtained when estimated vapor pressure data is used with the default option. A small sampling of compounds (37) indicates for most straight chain (4 to 5 or less) hydrocarbons, alcohols and ketones, relative error will be around 5% or less. For branched hydrocarbons, the relative errors may be in the range of 10% or less.

**Example 1.** Use the Edmister technique to estimate the acentric factor for component 201 (201 is the component ID number).

**Coding:**

```
ACE (EDM) 201  
PC (LYD) 201  
TC (LYD) 201  
TB 201 = 219.2
```

#### ChemTran: PENG-Robinson Option for Acentric Factor

The user may also request calculation of an acentric factor resulting from fitting vapor pressure data to the Peng-Robinson equation.

**NOTE:** For non-standard components, TC, PC, TB and P-T commands are also required.

**Example 1.** Estimate an acentric factor by fitting vapor pressure data for component 200 to the Peng-Robinson equation.

**Coding:**

```
ACE (PEN) 200
PC 200 = 710.4
TC 200 = 552.22
P-T (C,MMHG) 200 = 60, 100, 450, 64, 6 50, 75.4, 760.4,
                    760, 80.14, 1000, 89.2
TB (C) 200 = 80.14
```

**ChemTran: SOAVE Option for Acentric Factor**

The user may request calculation of an acentric factor by fitting vapor pressure data to the SOAVE equation of state.

**NOTE:** for non-standard components, entries for TC, PC, TB and P-T are also required.

**Example 1.** Use vapor pressure data from the Data Base to generate acentric factor for the SOAVE equation of state for CO<sub>2</sub>, H<sub>2</sub>S, methane and ethane (component ID numbers 49, 50, 2 and 3, respectively).

**Coding:**

```
ACE (SOAVE) 49
ACE (SOAVE) 50
ACE (SOAVE) 2
ACE (SOAVE) 3
```

**ChemTran: APISOAVE Option for Acentric Factor**

The user may also supply a data input requesting calculation of the acentric factor by fitting vapor pressure data to the APISOAVE modified SOAVE equation of state. For non-standard components, entries for TC, PC, TB and P-T commands are also required.

**NOTE:** the acentric factors should not be recalculated for components for which interaction parameters are available in the APISOAVE technique. See *ChemTran: Table 1. APISOAVEK Interaction Parameter List* for the table of binary pairs contained in this technique.

**Example 1.** Use vapor pressure data from the Data Base to generate acentric factors for the API modification of the SOAVE equation for ethane and ethylene (component ID numbers 3 and 22, respectively). VLE data will be fitted to the APISOAVE equation.

**Coding:**

```
ACE (APISOAVE) 3
ACE (APISOAVE) 22
P-Y-X (C,ATM) 22, 3 = -17.8, 16.1, .15, .1, 17.4, 12837, .2, 20.8, .6, .5,
APISOAVEK
COM = 3,22
```

---

## ChemTran: Volume (Density) Methods

---

Liquid densities (or volumes) are calculated as required by default options in ChemTran by a density correlation. Best results are obtained if liquid density or volume data is supplied for the component with a V-T command via *ChemTran: Density Commands*. The calculation will proceed with a minimum of values for T<sub>c</sub> and P<sub>c</sub>.

**NOTE:** Units **must** be entered on the V-T command.

**Example 1.** Enter density data for component 200, where 200 is the component ID number. Data is valid over the temperature range of 50-100 F.

**Coding:** **v-T** (LB/FT<sup>3</sup>) 200 = 50, 150, 30, 60, 27.6, 97, 25,  
8, 23.8, 146

**Example 2.** Enter volume constants for component 201. Data is valid over the temperature range of 50 - 150 F.

**Coding:** **v-T** (FT<sup>3</sup> / LB, CON) 201 - 50, 150, .80497,  
-.92529E-3, .11946E-5

---

## ChemTran: Characteristic Volume Method

---

The definition of the characteristic volume is:

$$V_w = V(T_b) / (5.7 + 3T_b / T_c)$$

and it is used to estimate liquid volumes for a component when no volume versus temperature data are available. It is calculated as a default option in ChemTran when other appropriate physical property data are available.

There are several combinations of data that will result in a default calculation of V. This data must be placed in the input file with the appropriate commands. Table 7.14. gives a list of the data combinations with a comment on the commands to use. The reliability decreases as one proceeds down the table.

## Chapter 16

**Table 7.14.**  
Data Combinations Required  
for Vw Calculation

Data	Comment
liquid density or volume at Tb,Pc,Tc & Vc	Use TB,PC,TC and VC commands
liquid density or volume data, Tb,Pc,Tc, & Vc	Use V-T,TB,PC,TC and VC commands
Tb, Pc, Tc, and Vc	Use TB,PC,TC and VC commands
Tb, Pc, Tc	Use TB,PC and TC commands

### ChemTran: Latent Heat Methods

#### Latent Heat Versus Temperature

L-T (units,options) i = TLL,TUL,L1,T1,L2,T2,... datalist

This command is used to enter latent heat data (heat of vaporization) for curve fitting or constants for one of two equations. Latent heat data is used for calculating enthalpy of a liquid. The parameters are:

TLL = lower temperature limit for data

TUL = upper temperature limit for data

Option1	Other Data Required	Data List	Comments
DATa+	none	L(T1),T1, L(T2),T2, up to 50 L,T values	enter data for curve fitting to equation specified by option2. If only one data point is entered the Watson method will be used to predict the latent Heat.
CONstants	none	C1,C2,C3	enter constants for latent heat equations

#### Option2

#### Equation

L+ L = C1 + C2\*T + C3\*T2

L\*\*1/2 L\*\*1/2 = C1 + C2\*T + C3\*T2

+default, this option is assumed if the command is entered without an option.

*Example 1.* Enter the following latent heat data for component 205. The data is reasonable over a temperature range 10 F to 230 F. Use the first equation option.

L (BTU/LB)	T F
456.7	100.0
443.6	155.0
424.4	196.0

**Coding:** L-T (BTU/LB,DAT) 205 = 10.,230.,456.7,100.,443.6,155.,424.4,196.,

#### Notes on Latent Heat

If data IS regressed the C1, C2, and C3 constants would fit the equation:

$$L = C1 + C2*T + C3*T2$$

If data IS NOT regressed the latent heat for water will be calculated by the equation:

$$L = 18.02*(75.0573 - 4260.42*(1 - Tr)^{1/3} + 3798.8*(1 - Tr)^{2/3} + 1595.99*(1 - Tr)^{4/3})$$

For substances other than water, IF NO data is regressed, the latent heat is calculated by the equation:

$$L = [C1*(1 - Tr)/(1 - C2/Tc)]^{0.38}; C3 = 1.0$$

If **NO DATA** is regressed the constants have the following meaning:

C1 = latent heat at the normal boiling point calculated by one of the above equations.

C2 = Normal boiling point in absolute temperature units.

C3 = 1.0 (not used)

### ChemTran: Solubility Parameter Method

The solubility parameter,  $\delta$ , is a data correlation parameter used in the ChemShare program. It is calculated from the relation,



$$\delta_i = \{(\Delta H_{\text{vap}} - RT_b) / V\}^{1/2}$$

where  $\Delta H_{\text{vap}}$  and  $V$  are evaluated at  $T = T_b$ . ChemTran automatically determines  $\delta$  if heat of vaporization ( $L - T$ ) and liquid density ( $V - T$ ) data or estimates have been provided in the file by the user. Any of the options applicable to each of these quantities are applicable to their use in the calculation of  $\delta$ .

Alternatively, the solubility parameter may be entered directly with the command.

**SOL** i = data

where i is the component ID number. The solubility parameter must be entered in units of (CAL/CM<sup>3</sup>)<sup>1/2</sup>.

## ChemTran: Surface Tension Methods

Pure component surface tension data can be entered directly in ChemTran, or predicted by two different techniques. Data will be fit to an equation of the form

$$\sigma = C_1 (1 - T_1) C_2$$

where " $\sigma$ " is the surface tension and " $T_r$ " is the reduced temperature. The parameters  $C_1$  and  $C_2$  will be adjusted to fit the data. Alternatively, they can be entered directly.

Each of the techniques for estimating data may require other properties for the chemical as well as the chemical structure. These properties can be entered directly with ChemTran commands. However, if only the STRUcture command is used, ChemTran will try to estimate other required properties. If no predictive technique is selected ChemTran will use one of the two methods in the following order:

1. **ChemTran: Macleod - Sugden**
2. **ChemTran: Brock - Bird**

### ChemTran: Macleod - Sugden

This technique estimated surface tension for a component based on the parachor. This quantity is defined by the following equation:

$$\sigma^{1/4} = P(\rho_l - \rho_v)$$

where  $P$  is the parachor. The density term is approximated with the expression

$$(\rho_l - \rho_v) = \rho_b^l (1 - T_r / 1 - T_{br})^n$$

where  $\rho_b^l$  is the liquid density at the normal boiling point, and  $T_{br}$  is the reduced normal boiling point temperature. The value of  $n$  is different depending on the type of chemical. Values of  $P$  are calculated from the molecular structure of the chemical.

The method is applicable to a wide variety of chemicals and is preferred where hydrogen bonding can occur. These include saturated and unsaturated hydrocarbons and hydrocarbons with the groups.

-COO-	-CHO
-COOH	O
-OH	N
-NH <sub>2</sub>	S
-O-	P
-NO <sub>2</sub>	F
-NO <sub>3</sub>	Cl
-CO(NH <sub>2</sub> )	B
=O	I,

and many types of ring compounds. ChemTran will automatically process a chemical structure to determine if this method can be applied.

### ChemTran: Brock - Bird

The Brock-Bird technique for surface tension is based on a corresponding states analysis. It requires values for  $T_c$ ,  $P_c$  and  $T_b$ . These can be input directly into ChemTran or estimated for the component using the STRU command. It is comparable to the Macleod - Sugden technique for many chemicals but is not suited for chemicals exhibiting strong interactions.

## ChemTran: Pure Component Required Commands

There are commands and options for each of the properties. However, not all of these commands are required. The following is a summary of the required commands for setting up the physical properties of a chemical; where i is the component ID

## Chapter 16

number (see *ChemTran: Entering Properties to Define a Custom Component*):

<b>Required Command</b>	<b>Purpose</b>
<b>COM</b> = i,j,k	component ID number list
<b>NAM</b> i =	name
<b>MOL</b> i =	molecular weight
<b>TB</b> (units, options) i =	normal boiling point
<b>TC</b> (units, options) i =	critical temperature
<b>PC</b> (units, options) i =	critical pressure
<b>VC</b> (units, options) i =	critical volume
<b>CP-T</b> (units, options) i =	ideal gas capacity

From this input ChemTran can predict vapor pressure, saturated liquid volume and the heat of vaporization. The remaining derived parameters - solubility parameter, acentric factor and characteristic volume - can then be calculated. The properties indicated in the minimum set of commands can be entered as data or as the structure of the chemicals. For a large class of chemicals all of these properties can be estimated from the structure with the single command STRUcture i =.

### ChemTran: Pure Component Optional Commands

In addition to the minimum set of commands listed above there are the following:

<b>Optional Commands</b>	<b>Purpose</b>
<b>P-T</b> (units, options) i =	vapor pressure
<b>V-T</b> (units, options) i =	liquid volume
<b>L-T</b> (units, options) i =	latent heat
<b>ACE</b> (options) i =	acentric factor
<b>SOL</b> (options) i =	solubility parameter
<b>SUR TEN-T</b> (units, options) i =	surface tension
<b>THE CONL-T</b> (units, options)	liquid thermal conductivity
<b>THE CONV-T</b> (units options) i =	vapor thermal conductivity
<b>VISL - T</b> (units options) i =	liquid viscosity
<b>VISV - T</b> (units options) i =	vapor viscosity
<b>ASS PAR</b> (units) i =	association parameters
<b>DIP MOM</b> (units) i =	Dipole moment
<b>PARA</b> (9units) i =	Parachore

These additional commands and the minimum set of commands provide a way of entering all of the physical properties of a chemical needed by DESIGN II.

**NOTE:** For solid components (300-399 ID numbers), HS-T, MOL and VS-T data must be entered.

#### Errors

Error evaluations are of primary importance in preparing a strategy for estimating a complete set of physical property data. The descriptions contain detailed error analyses obtained from original literature references for each method employed. These analyses should serve as a guide in selecting estimation techniques.

However, in order to obtain a dependable estimate of errors for a chemical, it is advisable to use the same set of techniques for a similar chemical or set of chemicals where reliable data are available. The simple input system of ChemTran greatly facilitates these evaluations.

### ChemTran: Unified Group Contribution Technique

ChemTran has the capability to predict several physical properties from a single structure input command. In addition, UNIFAC can be used to predict V-L-E data with the same command. This command unifies all group contribution tables for each property. This technique is applicable to hydrocarbon molecules containing at least two carbon atoms.

The command requires only a knowledge of the structure of bonding in the molecule. Coding of a structure requires three steps:

- Write down the structural formula of the molecule;
- Number all non-hydrogen atoms (It is not necessary to include information for any of the hydrogen atoms);
- Enter the bonding using the following command

**STRU**cture i = bonding data (where i is the component ID number).

Symbols which are permitted for the structure are:

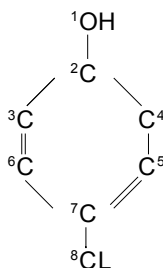
<b>Type</b>	<b>Bonds</b>	<b>Symbol</b>
single bond		-
double bond		=
triple bond		*

#### Atomic Symbols

Atom	Symbol
Boron	B
Bromine	BR
Carbon	C
Chlorine	CL
Fluorine	F
Hydrogen	H
Iodine	I
Nitrogen	N
Oxygen	O
Silicon	SI
Sulfur	S

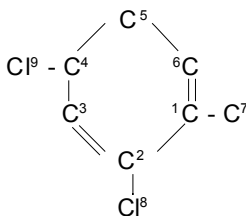
The bonding data required to describe the chemical structure is illustrated in several examples which follow. After ChemTran has processed the structure data and generated physical properties, a drawing of the structural formula will be provided as a check on the bonding information which was entered.

**Example 1.** Enter the bonding structure for 4-chlorophenol



STRUcture 201 = C2 - O1, C2=C4, C4 - C5 C2 - C3,  
C3 = C 6, C6 - C7, C7 - CL8, C7 = C5

**Example 2.** Enter the structure for 2,4-dichlorotoluene



#### Coding:

```
*SAMPLE OF PURE COMPONENT DATA GENERATION
COMPONENT = 200
STRUCTURE 200 = C1-C2,C2=C3,C3-C4,C4=C5,C5-C6,C6=C1,C1-C7,
                C2-CL8,C4-CL9
RENON K
LATENT HEAT
NAM 200 = 2-4 DICHLOROC7H8
FIL NEW = 2-4,DICL,C7H8
END
```

### ChemTran: Application of the Structure Command

The STRUcture command greatly simplifies the use of ChemTran for prediction of physical properties. In fact, if only the structure command is entered, ChemTran will label the compound, calculate its molecular weight, and attempt to predict all the physical and thermodynamic properties needed by DESIGN II such as:

- *boiling point*
- *critical temperature, pressure and volume*
- *ideal gas heat capacity*
- *vapor pressure*
- *acentric factor*
- *density*
- *characteristic volume*

## Chapter 16

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- *latent heat*

ChemTran will automatically select a technique for property prediction from the following hierarchical list:

### Boiling point

Stiel and Thodos  
Ogata and Tsuchida  
Lydersen, Forman and Thodos

### Critical temperature

Lydersen  
Forman and Thodos

### Critical pressure

Lydersen  
Forman and Thodos

### Critical Volume

Lydersen  
Yen-Wood (requires a liquid density point entered with a V-T command)

### Ideal Gas Heat Capacity

Benson  
Parr

The preferred method is always the first on the list. If the method is not applicable, ChemTran will automatically try the next method on the list. If none of the methods are applicable, then appropriate error messages will be printed.

The user can also request a specific technique by entering the appropriate keyword command for the property and option desired plus the component ID number. Although ChemTran can predict properties necessary for DESIGN II, it is always better to enter as much experimental data as possible. All pure component commands are compatible with the STRUcture command. For example, if a boiling point is entered for a component, ChemTran will bypass the boiling point estimation.

The following is a sample input combining the STRUcture command with other ChemTran pure component commands.

**Example 1.** Set up the property data for a mixture of ethanol and isopropyl propyl ether. Since isopropyl propyl ether is not in the Data Base, some properties need to be estimated. From the [Handbook of Chemistry and Physics](#).

boiling point is 83° C  
density is .7370 g/cm<sup>3</sup> at 20° C

$$\begin{array}{c} \text{C}^1 \\ | \\ \text{C}^2 - \text{O}^4 - \text{C}^5 - \text{C}^6 - \text{C}^7 \\ | \\ \text{C}^3 \end{array}$$

The structure for isopropyl propyl ether is

### Coding:

```
*METHANOL AND ISOPROPYL PROPYLEETHER
COMPONENTS = 1021, 200
NAME 200 = ISO-PROPYL-ETHER
TB (C) 200 = 83.
V-T (C,G/CM3) 200 = 19.,21., .7370, 20,
STRUCTURE 200 = C1-C2,C2-C3,C2-04,04-C5,
                C5-C6,C6-C7
END
```

---

## ChemTran: UNIFAC Estimation Technique for Activity Coefficients

---

UNIFAC is a method for estimating activity coefficients for binary pairs based on the group-contribution concept. It can be used in ChemTran to calculate binary interaction parameters to fit any of the RENon, WILson, or UNIQUAC equations see *ChemTran: K-Value Options* and *ChemTran: Correlating Mixture Data*. UNIFAC estimates are based on parameters that have a one-to-one correspondence to the functional groups, also known as UNIFAC groups, in mixture components and group interactions between the UNIFAC groups. In order to use the UNIFAC technique, the structure for each component must be defined in terms of UNIFAC groups. The structure of all database components are available to the UNIFAC method. Non-standard component structures are entered with the structure command.

ChemTran automatically determines which UNIFAC groups are present and calculates the infinite dilution activity coefficient.

If you want to enter a structure for a non-standard component or override a database structure you would use the STRUcture command.





## ChemTran Command Summary

### ChemTran File Access Commands

#### File Creation

FILE **NEW** = name 1, name 2, name 3

#### File Usage, Maintenance, and Deletion

FILE **OLD** = name 1, name 2, name 3, key

### DESIGN II File Access Commands

DESIGN II gains access to this data via a CHEmtran FILE command. The file names used in DESIGN II must be the same names used in ChemTran when the file was created.

CHEmtran FILE = name1,name2,name3

### Electrolyte Commands

#### EDWARDK

ION **COM**ponents = 9401,...,9999

ION **NAME** i =

IONic **FOR**mula i = # of atom1 \* atom1, # of atom2 \* atom2,....

IONic **CH**arge i = value

LIBrary **REA**ction = 101,101,... 1,2,....

**REA**ction **STO**ichiometry i = (a1\*r1 + a2\*r2 + ..... = b1\*p1 + b2\*p2 + .....)

**EQU**ilibrium **CON**stant (units) i = TLL, TUL, A, B, C, D

**EDA** i,j = Aij, Aji, Bij, Bji, Cij, Cji

**EDB** i,j = Dij, Dji

**HEN**ry's constant in **WAT**er (options, units) i = TLL,TUL,....

Two of the following options are available for HEN WAT command.

**DATA**

**HEN WAT** (DAT,units) = TLL,TUL,H1,T1,H2,T2,....

**CON**stants

### Pure Component Properties Required Commands

**NAME** i =

**COM** = i,j,k,....

**TC** (units,options) i = data list

**PC** (units,options) i = data list

**VC** (units,options) i = data list

**CP-T** (units,options) i = TLL,TUL,data list

**MOLE**cular weight i = data list

**TB** (units,options) i = data list

**AMB** (units) i =

**API** (units) i =

**AMW** i =

### Pure Component Properties Optional Commands

**ACE**ntric factor (option) i =

**V-T** (units,options) i = TLL,TUL, data list

**VS-T** (units,options) i = TLL,TUL, data list

**HL-T** (units,options) i = TLL,TUL,data list

**HV-T** (units,options) i = TLL,TUL,data list

**HS-T** (units,options) i = TLL,TUL,data list

**KMODPEN** (option) i =

**K-T** (units,options) i = limits, data list

**L-T** (units,options) i = TLL,TUL,L1,T1,L2,T2,.... data list

**CPL-T** (units,options) i = TLL,TUL,CPL1,T1,CPL2,T2,.... data list

**SUR TEN-T** (units, option) i = TLL,TUL,data list

**PRI PRO**

**TABLE X-T**(units) i = initial T, final T, number of degrees per increment

**THE CONL-T**(units,options) i = TLL,TUL, data list

**THE CONV-T**(units,options) i = TLL,TUL, data list

**VISL-T**(units,options) i = TLL,TUL, data list

**VISV-T**(units,options) i = TLL,TUL, data list

**STRU**cture i = bonding data (where i is the component ID number).

**P-T** (units,options) i = TLL,TUL,P1,T1,P2,T2,...data list

**ASS**ociation **PAR**ameter i =

## Chapter 16

DIPole MOMent i =  
PAR i =

**ChemTran Output Units System**  
AMERican UNIts OUT  
SI UNIts OUT  
METric UNIts OUT

### ChemTran: Mixture Commands Summary

This section summarizes commands for entering, correlating, and predicting mixture data for K-values, enthalpies, and densities. There are six categories of commands. One or more commands may be selected from each category to

1. select thermodynamic correlations
2. enter binary interaction parameters
3. enter infinite dilution activity coefficients
4. enter VLE, LLE, and heat of mixing data
5. select correlation options for VLE and LLE data
6. graph binary VLE data from correlations

VLE and LLE commands for the same mixtures will be regressed simultaneously. This simplifies data entry for cases where:

- 1.) data with different input units is entered, or
- 2.) data for binary, ternary and higher are entered in the same input file

More importantly, ChemTran permits simultaneous regression of VLE, LLE, and VLLE data. This feature is necessary in order to obtain a good thermodynamic model for VLLE behavior.

The following table summarizes these commands. These will be listed in alphabetical order.

#### TABLE OF INPUT COMMANDS FOR MIXTURES

##### Selection of Thermodynamic Correlations:

APIISOAVE K  
IDEal VAPor  
PENg K  
RENon  
SOAVE K  
WILson  
UNIQUAC K  
UNIFAC K  
HAYDen O'CONell VAPor  
CHEmical THEory VAPor

##### Entry of Binary Interaction Parameters:

APIISOAVE (units)  $i, j = A_{ij}, B_{ij}$   
IDE(units)  $i, j$   
MARGules (units)  $i, j = T, A_{ij}, A_{ji}$   
PENg (units)  $i, j = A_{ij}, B_{ij}$   
RENON (units)  $i, j = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}, C_{ij}$   
SOAVE (units)  $i, j = A_{ij}, B_{ij}$   
UNIQUAC (units)  $i, j = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}$   
VAN laar (units)  $i, j = T, A_{ij}, A_{ji}$   
WILson (units)  $i, j = T, A_{ij}, A_{ji}, B_{ij}, B_{ji}$   
MOD PEN  $i, j = A_{ij}, A_{ji}, B_{ij}, B_{ji}$   
MODified PENg K

FIX  $i, j =$  data list  
VARY  $i, j =$  data list

GRAph variable 1 - variable 2 (options, units)  $i, j =$  data  
This Permits four types of graphs:

<u>Command</u>	<u>Function</u>
GRAph Y-X	Y vs. X at constant T or P
GRAph T-X	T vs. X at constant P



GRAph P-X                    P vs. X at constant T  
 GRAph A-X                     $\gamma$  vs. X at constant T or P

**Entry of Infinite Dilution Activity Coefficients:**

**ACT**ivity (units, DATA)  $i,j = T1, \gamma_i, \gamma_j$

**ACT**ivity (units, **UNIFac**)  $i,j = T$

**SCA**tchard Hildebrand

**Entry of VLE, LLE, or Heat of Mixing Data:**

**P-X** (units)  $i,j,\dots,n = T1, P1, X1i, X1j,\dots, X1n-1,$

**P-Y-X** (units)  $i,j,\dots,n = T1, P1, Y1i, Y1j,\dots, Y1n-1, X1i, X1j,\dots, X1n-1,$

**P-Y-X-X** (units)  $i,j,\dots,n = T1, P1, Y1i, Y1j,\dots, Y1n-1, X11i,$   
 $X11j,\dots, X11n-1, X21i, X21j,\dots, X21n-1,$

**T-P-X** (units)  $i,j,\dots,n = T1, P1, X1i, X1j,\dots, X1n-1,$

**T-P-Y-X** (units)  $i,j,\dots,n = T1, P1, Y1i, Y1j,\dots, Y1n-1, X1i, X1j,\dots, X1n-1,$

**T-P-Y-X-X** (units)  $i,j,\dots,n = T1, P1, Y1i, Y1j,\dots, Y1n-1,$   
 $X11i, X11j,\dots, X11n-1, X21i, X21j,\dots, X21n-1,$

**T-X** (units)  $i,j,\dots,n = P, T1, X1i, X1j,\dots, X1n-1,$

**T-X-X** (units)  $i,j,\dots,n = P, T1, X11i, X11j,\dots, X11n-1, X21i, X21j,\dots, X21n-1,$

**T-Y-X** (units)  $i,j,\dots,n = P, T1, Y1i, Y1j,\dots, Y1n-1, X1i, X1j,\dots, X1n-1,$

**T-Y-X-X** (units)  $i,j,\dots,n = P, T1, Y1i, Y1j,\dots, Y1n-1, X11i,$   
 $X11j,\dots, X11n-1, X21i, X21j,\dots, X21n-1,$

**HE-T-X** (units)  $i,j = He1, T1, X1i, He2, T2, X2i,$

## ChemTran Step by Step

The ChemTran input file contains all the keyword commands necessary to enter, regress, or estimate the desired physical property and thermodynamic data. The input file must be an ASCII text file and can be created when under the DESIGN II main menu Simulate---Use ChemTran Option---DESIGN II Input Manager Window or with an ASCII text editor. The following is a step-by-step guide on how to build a ChemTran input file. The first step, entering your DESIGN II account number, is mandatory and must be first. All other steps may be done in any order you choose and most are not mandatory.

### ChemTran STEP 1

Enter your DESIGN II account number. This is mandatory and must be on the first line of the input file and begin in the left hand column.

*Example:*            **AB123.**

### ChemTran STEP 2

Enter title for ChemTran file. This title will appear on the top of each page of the output. This step is not mandatory, however, if a title command is entered it must be on the second line of the input file.

*Example:*            \* Pure Component Data Inclusion and Regression of WATER ETHANOL DATA

### ChemTran STEP 3

Identify the components to be included in the ChemTran file. A list of component numbers may be found in *Database Components* This command is mandatory, although it may appear anywhere in the input file

*Example:*        COMponents = 200,1012,40,41

### ChemTran STEP 4

Enter pure component commands see *ChemTran: Pure Component Command Details*. These commands are optional and may be located anywhere in the input file

*Example:*

```
NAM 200 =Non-Database Chemical Component
MOL 200 = 114.22
TB (C) 200 = 113.47
TC (F) 200 = 559.47
PC (ATM) 200 = 26.94
P-T (C,MMHG) 200 = 36.57,300.0,47.71,36.57,760,113.47 20473.9,293.04
VC (FT3/LBMOL) 200 = 7.38
CP-T (R,DAT,T**3) 200 = 500,2800,45.35,540,57.52,720,68.22,900,
L-T (BTU/LB,F,DAT,L**1/2) 200 = 65,260,144.52,68,133.04,158,
V-T (FT3/LBMOL,K) 200 = 300,550,2.7134,311.4,2.8242,360
```

## Chapter 16

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### ChemTran STEP 5

---

Enter mixture Commands see *ChemTran: Mixture Command Details* of the ChemTran User's Guide. These commands are optional and may be located anywhere in the input file.

*Example:*

C-VAPOR-LIQUID EQUILIBRIUM DATA FOR COMPS. 1021 AND 40

```
T-Y-X (C,MMHG) 1021,40=760,  
70.67, .2670, .0260,  
66.44, .3710, .0500,  
62.87, .4570, .0880,  
60.20, .5260, .1640,  
58.64, .5590, .3330,  
58.02, .5950, .5490,  
58.10, .6330, .6990,  
58.47, .6650, .7820,  
59.90, .7600, .8980,  
62.71, .9070, .9730
```

C- K-VALUE OPTION  
WILSON

---

### ChemTran STEP 6

---

Enter Chemical File Commands. The FILE NEW command instructs ChemTran to create the property file that interfaces the ChemTran results with DESIGN II. The interface file allows DESIGN II to use the thermodynamic and physical properties entered into ChemTran with its process models. The interface file is referred to as the 'Chemical File'.

**FILE NEW** = name1,name2,name3,

**FILE OLD** = name1,name2,name3, key

Where the key controls how the ChemTran operates on the existing chemical file.

<u>Key</u>	<u>ChemTran Operation</u>
0	Reads the existing file
2	Reads the existing file; then erases it; then writes a new file.
3	Writes on an old file
4	Erases the existing, removes VLE commands from input file before execution.

**NOTE:** Only one Chemical File can be accessed or written in a ChemTran run.

*Example:*     **FILE NEW** = MEOH,WATR,DATA  
C-     **FILE OLD** = MEOH,WATR,DATA,3

---

### ChemTran STEP 7

---

Enter the **END** command to terminate the input file. This command is mandatory and must appear on the last line in the input file.

```
AB123.  
*CHEMTRAN DEMONSTRATION  
COM=200,204,1021,40  
C-NON-DATABASE COMPONENT NAMES  
C-  
NAM200=2.3.4-TRI-C1-C5  
NAM204=2.3.3-TRI-C1-C4  
C-  
C-PURE COMPONENT DATA FOR COMPONENT 200  
MOL 200=114.22  
TB (C) 200=113.47  
TC (F) 200=559.47  
PC (ATM) 200=26.94  
P-T (C,MMHG) 200=36.57,300.0,47.71,36.57,760,113.47,20473.9,293.04  
VC (FT3/LBMOL) 200=7.38  
CP-T (R,DAT,T**3) 200=500,2800,45.35,540,57.52,720,68.22,900,  
77.56,1080,85.65,1260,92.6,1440,98.52,1620,  
103.51,1800,107.7,1980,111.1,2160,114.07,  
2340,116.47,2520,118.5,2700  
L-T (BTU/LB, F, DAT, L**1/2) 200=65,260,144.52,68,133.04,158,139.93,  
104,135.32,140,130.73,176,126.14,212,121.55,248  
V-T (FT3/LBMOL, K) 200=300,550,2.7134,3111.4,2.8242,360.05,  
2.9349,424,3.0457,481.25,3.1564,537.85  
C-  
C-STRUCTURE FOR COMPONENT 204  
STRU 204=C1-C2,C2-C3,C3-C4,C2-C5,C2-C6,C3-C7  
C-
```

```

C-VAPOR-LIQUID EQUILIBRIUM DATA FOR COMPS. 1021 AND 40
C-
T-Y-X(C,MMHG) 1021,40=760,70.67,.2670,.0260,66.44,.3710,.0500,
        62.87,.4570,.0880,60.20,.5260,.1640,58.64,.5590,.3330,
        58.02,.5950,5490,58.10,.6330,.6990,58.47,.6650,.7820,
        59.90,.7600,.8980,62.71,.9070,.9730
C-
C-GRAPH COMMANDS FOR V-L-E PLOTS
GRA Y-X(C) 1021,40=60
GRA T-X(MMHG) 1021,40=760
GRA P-X (C) 1021,40=60
GRA A-X(C) 1021,40=60

C-K-VALUE OPTION WILSON
C-GENERATE WILSON PARAMETERS FROM UNIFAC
ACT(C,UNIFAC) 1021,200=60
ACT(C,UNIFAC) 1021,204=60
ACT(C,UNIFAC) 40,200=60
ACT(C,UNIFAC) 40,204=60

C-USE REGULAR SOLUTION THEORY TO CALCULATE
C-ALL OTHER BINARY INTERACTIONS (SCAatchard Hildebrand)
C-
C-CREATE DESIGN II INTERFACE FILE
C-
FILE NEW=CHEM,FILE,DATA
END

```

## ChemTran Examples

There are many more sample input files in "Chapter 7: ChemTran Samples - c:\designii\samples\chemtran" of the DESIGN II for Windows Tutorial and Samples Guide.

### ChemTran: Guidelines for Regressing Equilibria Data

(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn1.in to simulate this problem)

Regressing equilibria data with ChemTran is often necessary in order to model chemical systems that exhibit non-ideal behavior. The following guidelines are presented to help you obtain the best possible data regressions.

#### Step 1 Find Data

Locate equilibria data for all binary pairs in your mixture. If data is unavailable for some of the binary pairs, you may consider using UNIFAC or Regular Solution Theory to estimate infinite dilution activity coefficients.

#### Step 2 Select Input Commands for Data

Decide what ChemTran Mixture Commands should be used to enter the data into your input file. See *ChemTran: Correlating Mixture Data* for further details.

#### Step 3 Select Objective Function

Select the objective function for your regression. The default objective function is the sum of the K-values. This is good for most situations. See *ChemTran: Table 6.2. Objective Functions for reduction of VLE data*.

#### Step 4 Select Thermodynamic Correlation

Decide which thermodynamic correlation the data will be regressed to. The available choices are presented in *ChemTran: K Value Options*. A general guideline to follow is that an equation of state should be selected for non-condensable gases and an activity coefficient method is suitable for liquid phase systems at low pressures. If your data includes two liquid phases your only choices are RENON or UNIQUAC.

Often times you will have several correlations that are suitable. If you are seeking the highest degree of accuracy you can consider regressing the data to several correlations in order to see which correlation provides the best data fit.

#### Step 5 Do preliminary Regression

Regress the data using the default interaction parameter calculations. The default calculations fit the data by calculating the 'A' interaction parameters such that the objective function is minimized. The 'B' parameters are set to zero. See the following input file and selected output.

ChemTran Input Default - Fit A interaction Parameters, B parameters Fixed to 0

```

AB123.
*VLE/LLE DATA REGRESSION
COM=71,62

T-X(MMHG,C) 62,71=760,

```

## Chapter 16

```
152.30, 0.000,  
146.30, 0.0100,  
96.40, 0.0550,  
95.00, 0.0810,  
95.20, 0.9800,  
96.70, 0.9850,  
98.00, 0.9960,  
99.30, 0.9980,  
100.00, 1.0000,  
UNIQUACK  
END
```

Selected Portions of ChemTran Output

```
* * * *REDUCTION OF PHASE EQUILIBRIUM DATA FOR SYSTEM 1 * * * *  
          COMPONENTS IN SYSTEM 1  
NO.      CODE NO.      NAME  
-----  
1         71 I-C3-BENZENE  
2         62 WATER
```

```
EQUATION OPTION IS UNIQUAC NUMBER OF ITERATIONS= 20  
SUM OF SQUARES OF THE OBJECTIVE FUNCTION= 0.1055281E 00  
STANDARD ERROR OF ESTIMATE= 0.8121273E-01  
ROOT MEAN SQUARE OF ERROR= 0.7656810E-01
```

```
CHEMSHARE CORRELATION CONSTANTS FOR ALL BINARY PAIRS  
FROM UNIQUAC EQUATIONS (BTU/LBMOL)  
          DATA          AVE TEMP  
BINARY PAIR  ORIGIN  CONSTANT  VALUE      (F)  
-----  
I-C3-BENZENE(71)+  
WATER (62)   DATA    A(71,62)   3195.31 227.84  
              A(62,71)   -586.948
```

### Step 6 Evaluate the Quality of the Regression

Once you have executed ChemTran evaluate the quality of your data fit by examining the output value labeled 'STANDARD ERROR OF ESTIMATE'. This is the standard deviation of the error of the objective function and is a measure of how well the correlation was fit to the data. It is desirable to have a standard error of estimate near 5% (.05), however, a greater error may be acceptable. In the case shown in Step 5 the standard error of estimate is 8.13%.

### Step 7 Improve Data Fit

If you require a better data fit than what was obtained in the preliminary regression, you will want to take steps to improve the data fit. The options you can consider are:

- Regress the data to another thermodynamic correlation
- Fit the temperature dependent 'B' parameters
- Select a different data set to regress
- Discard data points that are inconsistent with the regression

The following ChemTran input file and selected output demonstrates how to fit the B parameters to the data.

```
AB123.  
*VLE/LLE DATA REGRESSION  
COM=71,62  
C-  
C- VARY B PARAMETERS  
VARY 62,71=B12,B21  
C-ENTER STARTING GUESSES FOR A PARAMETERS FROM PRELIMINARY REGRESSION  
UNIQUACK (BTU/LBMOL,F) 71,62=227.84,3195.31,-586.958  
T-X (MMHG,C) 62,71=760,  
152.30, 0.0000,  
146.30, 0.0100,  
96.40, 0.0550,  
95.00, 0.0810,  
95.20, 0.9800,  
96.70, 0.9850,  
98.00, 0.9960,  
99.30, 0.9980,  
100.00, 1.0000,  
UNIQUACK  
END
```

Selected portions of ChemTran output.

```
* * * *REDUCTION OF PHASE EQUILIBRIUM DATA FOR SYSTEM 1 * * * *  
          COMPONENTS IN SYSTEM 1  
NO.      CODE NO.      NAME
```

```

-----
1          71 I-C3-BENZENE
2          62 WATER

```

```

EQUATION OPTION IS UNIQUAC
NUMBER OF ITERATIONS=
47 SUM OF SQUARES OF THE OBJECTIVE FUNCTION= 0.270569E-02
STANDARD ERROR OF ESTIMATE= 0.1390193E-01
ROOT MEAN SQUARE OF ERROR= 0.1226035E-01

```

```

CHEMSHARE CORRELATION CONSTANTS FOR ALL BINARY PAIRS
FROM UNIQUAC EQUATIONS (BTU/LBMOL)

```

BINARY PAIR	DATA ORIGIN	CONSTANT	AVE TEMP VALUE (F)
-----			
I-C3-BENZENE (71)+			
WATER (62)	DATA	A (71, 62)	24061.3 227.84
		A (62, 71)	-1655.94
		B (71, 62)	-14.6924
		B (62, 71)	0.573410

Fitting the B parameters in addition to the A parameters resulted in the data fit improving from 8.12% to 1.39%.

---

## ChemTran: Entering Properties to Define a Custom Component

---

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open... c:\designii\samples\chemtran\chemtrn2.in to simulate this problem)**

The following input file illustrates how ChemTran can be used to define properties for a component not included in the DESIGN II or ChemTran component database. There are 7 commands required to define a custom component. If the following commands are entered, all other thermodynamic and physical properties can be calculated. Although the following input file defines the minimum set of commands necessary to define a custom component, you may enter data for any of the properties listed in *ChemTran: Pure Component Command Details*.

```

AB123.
*CHEMTRAN DEMONSTRATION
COM=200
C-NON-DATABASE COMPONENT NAMES
C-
NAM200=2.3.4-TRI-C1-C5
C-
C-PURE COMPONENT DATA FOR COMPONENT 200
C-ENTER MOLECULAR WEIGHT, NORMAL BOILING POINT,
C-CRITICAL TEMPERATURE, CRITICAL PRESSURE,
C-VAPOR PRESSURE DATA, CRITICAL VOLUME,
C-AND IDEAL GAS HEAT CAPACITY DATA
MOL 200=114.22
TB (C) 200=113.47
TC (F) 200=559.47
PC (ATM) 200=26.94
P-T (C,MMHG) 200=36.57,300.0,47.71,36.57,760,113.47,
20473.9,293.04
VC (FT3/LBMOL) 200=7.38
CP-T (R,DAT,T**3) 200=500,2800,45.35,540,57.52,720,68.22,900,
77.56,1080,85.65,1260,92.6,1440,98.52,1620,
103.51,1800,107.7,1980,111.1,2160,114.07,
2340,116.47,2520,118.5,2700
FILE NEW = 234T,CHEM,DATA
END

```

---

## ChemTran: Entering Data for Pseudo Components (100) and Chemical Components (200)

---

Input file showing data entry for Pet-100 (pseudo components) and Chem-200 (chemical) level components for inclusion in DESIGN II database.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open... c:\designii\samples\chemtran\chemtrn3.in to simulate this problem)**

```

AB123.
*CHEMICAL COMPONENTS--CHARCOAL, ASH, & CARBON (200 LEVEL)
*AND PSEUDOCOMPONENT(100-104)

C- CHAR, ASH, AND CARBON
COM=1,2,3,22,40,46,47,48,49,50,62,63,200,201,202
100,101,102,103,104

```

# Chapter 16

---

```
STDK
LAT
C-FILE NEW=ASH,CHAR,DATA

C-*****CHAR*****
MOL 200=12
NAM 200=CHAR
STRU 200=C1=C2
TB (F) 200=-200
TC (F) 200=-100
PC (PSIA) 200=125
VC 200=
SOL 200=1
CP-T (K) 200=200,2000,1.8,298,2.7,400,3.15,500,3.68,600,
    3.96,700,4.27,800,4.74,1000,5.04,1200,5.34,1400
    5.80,1600
K-T (CON,R) 200=50,5000,.1E-6,0.0,0.0
L-T (BTU/LBMOL,F) 200=0,2500,0.0001,100,0.0001,1000,0.0001,2500
V-T (LBMOL/FT3,F) 200=0,2500,8.3333,0.,8.3333,2500,8.3333,-200

C-*****ASH*****
MOL 201=116
NAM 201=ASH
STRU 201=SI1-C2,C2=O6,SI1-C3,SI1-C4,C4=O7,SI1-C5
TB (F) 201=-200.
TC (F) 201=-100.
PC (PSIA) 201=1622.8
VC 201=
SOL 201=1.0
CP-T (K) 201=200,2000,21.37,298,23.23,400,24.85,500,26.36,600,
    28.11,700,29.73,800,32.98,1000,36.24,1200,39.49,1400,
    41.50,1600
K-T (CON,R) 201=50,5000,0.1E-6,0.0,0.0,
L-T (BTU/LBMOL,F) 201=0,2500,0.0001,0,0.0001,1000,0.0001,2500
V-T (LBMOL/FT3,F) 201=0,2500,1.5603,0,1.5603,1000,1.5603,-200

C-*****CARBON*****
NAM 202=CARBON
MOL 202=12.01
STRU 202=C1=C2
TB (F) 202=-200.
TC (F) 202=-100.
PC (PSIA) 202=1216.7
VC (FT3/LBMOL) 202=1.25
SOL (CAL/CM3) 202=1.0
K-T (CON,R) 202=50,5000,0.1E-6,0.0,0.0,
L-T (BTU/LBMOL,F) 202=0,2500,0.0001,0,0.0001,1000,0.0001,2500
V-T (LBMOL/FT3,F) 202=0,2500,11.698,0,11.698,1000,11.698,-200
CP-T (K) 202=200,2000,2.038,298,2.85,400,3.5,500,4.04,600,
    4.44,700,4.74,800,5.15,1000,5.43,1200,5.61,1400,
    5.72,1600

C-*****LIGHT OIL 1*****
API (API) 100=3.0
AMW 100=112
AMB (F) 100=350.
NAM 100 =LIGHT OIL1

C-*****LIGHT OIL 2*****
API (API) 101=-10.5
AMW 101=175
AMB (F) 101=555.
NAM 101=LIGHT OIL2

C-*****LIGHT OIL 3*****
API (API) 102=-14.4
AMW 102=215
AMB (F) 102=680.
NAM 102 =LIGHT OIL3

C-*****LIGHT OIL 4*****
API (API) 103=-17.9
AMW 103=305
AMB (F) 103=880.
NAM 103=LIGHT OIL3

C-*****LIGHT OIL 5*****
API (API) 104=-19.3
```

```
AMW 104=410
AMB (F) 104=170.
NAM 104=LIGHT OIL5
```

```
END
```

---

## ChemTran: Entering Data for Solid Components (300)

---

Input file showing data entry for Chem-300 level (solid-carbon) component for inclusion in DESIGN II database.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn4.in to simulate this problem)**

```
AB123.
*DATA FOR CARBON as a solid

C- Components numbered 300-310 are allocated as solids by DESIGN II
COM=300

C- Name the component
NAM 300=CARBON

C- Volume of Solid data
VS-T (DATA) 300=0,2500,0.0854847,0,0.0854847,1000,0.0854847,-200

C- Molecular Weight data
MOL 300=12.01

C- Enthalpy of Solid data if available
HS-T (BTU/LBMOL,K) 300=200,2000,2.038,298,2.85,400,3.5,500,4.04,600,
  4.44,700,4.74,800,5.15,1000,5.43,1200,5.61,1400,5.72,1600

C- Include the following line for DESIGN II accessible data file
C- A file named 'carbonxx.dat' will be saved in the same sub-directory.

FILE NEW=CARB,ONXX,DATA
END
```

---

## ChemTran: Entering Experimental or Literature Values for Binary Interaction Parameters

---

Input file showing binary interaction parameter data entry for a component system using available correlations. No VLE/LEE data regression is needed.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn5.in to simulate this problem)**

```
AB123.
C- TRANS 2 BUTENE, DIMETHYL FORMAMIDE
COM = 26, 4136
RENON
RENON (BTU/LBMOL,F) 26,4136=122,2604.34,-180.706,0,0
FILE NEW = T2BT,DMFD,DATA
END
```

---

## ChemTran: Calculating Binary Interaction Parameters by Regressing VLE Data

---

Input file showing VLE data entry to back out binary interaction parameters based on a chosen non-ideal thermodynamic (Wilson) expression.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn6.in to simulate this problem)**

```
AB123.
*ACETONE-WATER
FILE NEW=DATA,ACET,H2O
WILSON K
C- ACETONE, WATER
COMP=1002, 62
C-
T-X-Y (MMHG,C) 1002,62=760, 76.25, .0490, .6050
  72.40, .0690, .6780
  66.45, .1270, .7530
  62.75, .2000, .7900
```

## Chapter 16

---

```
62.34, .2760, .8040
60.90, .3100, .8260
60.17, .4950, .8320
58.80, .6500, .8550
58.47, .6940, .8620
57.95, .7500, .8760
57.25, .8290, .9030
56.75, .9000, .9360
```

END

---

### ChemTran: Calculating Binary Interaction Parameters from Infinite Dilution Activity Coefficients

---

Input file showing a method to back out binary interaction parameters (any correlations) using infinite dilution activity coefficients of the binary. No VLE/LLE data required.

(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn7.in to simulate this problem)

```
AB123.
C- ETHANOL, DIETHEYL ETHER
COM= 1012, 1005
FILE NEW = ETHO,DETE,DATA
WILSON
ACT(C) 1005,1012 = 40,2.63,3.92
END
```

---

### ChemTran: Calculating Binary Interaction Parameters from Infinite Dilution Activity Coefficients Estimated from UNIFAC

---

Input file to back out binary interaction parameters using infinite dilution activity coefficients of the binary using UNIFAC (estimation method). No VLE/LLE data required.

(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn8.in to simulate this problem)

```
AB123.
C- ETHANOL, ACETONE
COM= 1012, 1002
FILE NEW = ETHO,ACET,DATA
WILSON
ACT(UNIFAC,C) 1002,1012 = 40
END
```

---

### ChemTran: Calculating Binary Interaction Parameters from Infinite Dilution Activity Coefficients using Regular Solution Theory

---

Input file to back out binary interaction parameters using infinite dilution activity coefficients of the binary using Regular Solution Theory. No VLE/LLE data required.

(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtrn9.in to simulate this problem)

```
AB123.
C- 1,3 BUTADIENE, 1 BUTENE
COM = 28,24
WILSON
SCA
FILE NEW = 13BD,1BUT,DATA
END
```

---

### ChemTran: Using the Structure Command to Define a Custom Component.

---

(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open...  
c:\designii\samples\chemtran\chemtr10.in to simulate this problem)

When part or all of the physical property data required to define a custom component is unavailable, you may wish to use ChemTran's group contribution methods to predict these properties. ChemTran's universal structure command is used to enter the molecular structure of the custom component and ChemTran will automatically determine what groups are present and predict all of the required physical properties. The following shows how the structure command is used to enter the component.

```
AB123.
*CHEMTRAN DEMONSTRATION
COM=204
```



```

C-NON-DATABASE COMPONENT NAMES
C-
NAM 204=2.3.3-TRI-C1-C4
C-C-STRUCTURE FOR COMPONENT 204
STRU 204=C1-C2,C2-C3,C3-C4,C2-C5,C2-C6,C3-C7
FILE NEW=233T,CHEM,DATA
END

```

---

## ChemTran: Using ChemTran to Output Component Physical Properties

---

Input file showing use of PRInt PROPERTIES command to print pure component properties in the DESIGN II/ChemTran database.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open... c:\designii\samples\chemtran\chemtr11.in to simulate this problem)**

```

AB123.
*PRINT PROPERTIES OF BENZENE
COM = 40
PRInt PROPERTIES
END

```

---

## ChemTran: Using the Modified Peng-Robinson Equation of State

---

Input file to fit data using Modified Peng-Robinson equation of state. This new method is applicable to non-ideal chemical systems at high pressure.

**(From the DESIGN II Menu Bar, please select...Simulate...Use ChemTran... Open... c:\designii\samples\chemtran\chemtr12.in to simulate this problem)**

```

AB123.
*WATER/CO2 REGRESSION WITH MODIFIED PENG ROBINSON
*METHOD
C-
C-      WATER CO2
COMPONENTS = 62, 49
C-
C- SPECIFY MODIFIED PENG ROBINSON EQUATION OF STATE
C- WITH MARGULES
C- MIX RULE
MODPENK (MAR)
C- SPECIFY REGRESSION OF KAPPA PARAMETERS FROM
C- LIBRARY VAPOR PRESSURE DATA
KMODPEN (VAP) 62
KMODPEN (VAP) 49
C-
C- REGRESS VLE DATA
C-
P-X-Y (BAR,K) 49,62=383.15, 99.999,.0140,.9560
      199.997,.0210,.9580
      299.995,.0240,.9480
      399.994,.0260,.9320
      499.992,.0280,.9140
      599.991,.0300,.8930
      699.990,.0315,.8720
      799.988,.0330,.8540
      899.986,.0345,.8400
FILE NEW = CO2,WATR,DATA
END

```

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# Chapter 17: Flowsheet Optimization

## Flowsheet Optimization Overview

Flowsheet Optimization is a powerful feature in DESIGN II to simplify a cumbersome and time-consuming process engineering task. Historically, process optimization required the user to submit numerous simulation runs in addition to initially converge the flowsheet simulation. The engineer's ultimate goal was to "fine tune" the process to optimize an important function. For each iterative rerun of the flowsheet simulation a key design variable would be altered until the design was designated "optimal"; more often than not because of a shortage of time. Now, the optimization procedure is automated. Simple key words are used to identify the design variables to be **VAR**ied to **MAX**imize or **MIN**imize the objective **FUN**ction, **SUB**ject **TO** the specified **CON**straints of the process.

While simulation solves a system with all the parameters specified, optimization searches for the optimal specification of the parameters. In other words, optimization deals with an under-specified system and tries to determine the values of the free parameters such that a prescribed function is optimized. The free parameters and the function to be optimized are called design variables and objective function, respectively. Often design variables are specified within certain physical bounds and system outputs are subject to certain design requirements. Such requirements are called constraints. For instance, the pressure range for a stream or maximum suction volume for a compressor represent some design limitations.

Optimization in a sequential modular simulator requires repeated module calculations according to a particular scheme. For DESIGN II, this scheme is built around an efficient **nonlinear programming (NLP)** algorithm. Specifically, the values of the design variables are updated from iteration to iteration according to simulation results, starting with a set of initial values, until some criteria for optimization are met. During each iteration, a search vector is first obtained from the local behavior of the objective function and constraints. Then a search is made along this vector for a new set of design variables which yields an improved objective function and constraint fulfillment.

## Flowsheet Optimization Command Details

### OPTIM Input Section

Flowsheet optimization in DESIGN II requires a special input section called OPTIMization. All the information related to an optimization problem, such as the choice of design variables, definition of objective function and constraints can be input in this section.

Only one OPTIMization section is allowed per run.

- The OPTIMization section may appear anywhere in the overall input after the title command and before the END command.
- The OPTIMization command must be the first command in this section. The OPTIM command requires a minimum of five characters.
- Comment commands, beginning with C- may appear anywhere within this section.
- Inline FORTRAN statements may be used to define constraint and objective functions. These statements may mingle with other optimization and comment commands in any order before the next equipment module or before the END statement. The order in which the Inline FORTRAN statements are entered will be maintained and they will be processed as a group.

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## Flowsheet Optimization Input Commands

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The **OPTIM**ization section has three types of commands:

```
VARy....SUBject TO....UNTil  
OPTimization TOLerance  
MAXimum ITEration
```

The last two commands are similar to other DESIGN II commands and perform the following functions:

**OPT**imization **TOL**erance =  
Set overall optimization tolerance.

**MAX**imum **ITE**rations =  
Set number of iterations.

These two commands can appear before or after the **VAR**y....**SUB**ject **TO**....**UNT**il commands and are optional.

The **VAR**....**SUB TO**....**UNT**.... commands provide a way of completely stating an optimization problem. Design parameters are contained in the **VAR**.... portion of the statement, constraints in the **SUB TO**.... portion of the statement, and the objective function in the **UNT**.... portion. Since the **SUB to**.... section is optional, **VAR**....**SUB TO**....**UNT**.... can reduce to **VAR**....**UNT**.... to state an optimization problem. Each of the sections, **VAR**...., **SUB TO**...., and **UNT**, has associated with it other input commands that may be necessary for the optimization. All of these optional commands are illustrated in the following general form of the **VAR**....**SUB TO**....**UNT**.... statement.

## Chapter 17

**VARy** (min1 **.LE.** var1 **.LE.** max1, **UNIT** = , **SCALE** = , **TOL** **ABS**  
or **REL** = , **PERT** **ABS**  
or **REL** = , **MAX STEP** = )

**AND**

(minn**.LE.** var n **.LE.** maxn ,**UNIT** = , **SCALE** = , **TOL** **ABS**  
or **REL** = , **PERT** **ABS**  
or **REL** = , **MAX STEP** = )

**SUBJECT TO**

**.LE**  
**OR**  
**.EQ** **EQ** constant 1 (**SCALE** = , **MULTIPLIER** = ),

**OR**

**.GE.**

**AND**

**.LE**  
**OR**  
**.EQ** constant k (**SCALE**= , **MULTIPLIER**= ),

or

**.GE.**

**UNTIL FUN** (**SCALE**= , **TOLERANCE** **ABS**  
or **REL** = ) **IS** **MAXIMIZED**  
or **MINIMIZED**

The **.LE.**, **.EQ.**, and **.GE.** are the FORTRAN equivalents of the "less than or equal to", "equal to", and "greater than or equal to" expressions. Only one of these expressions can be selected from the group **.LE.** or **.EQ.** or **.GE.**

All input commands summarized in this section are governed by the following rules:

- Characters shown in **bold face** are the minimum recognizable keywords which must be entered.
- All information about each design variable is enclosed by a pair of parentheses.
- Multiple design variables, if specified, must be separated from each other by a comma or **AND** expression.
- Although the optimization statement can be continued on as many lines as necessary, a new line must not begin with an equipment module identifier.
- Spaces may be entered at any position of the input.
- Commas are typically used to separate keyword phrases.
- The Inline FORTRAN convention of equipment module identifier, equipment number and equipment parameter keyword (including index, if parameter allows for multiple values) must be followed (i.e. module identifier (equipment number), parameter keyword (index position)). For example, the outlet pressure or **PREssure OUT** for **COMPRESSOR 35** would be defined as: (**COMPRESSOR (35), PREssure OUT**)
- The left-most and right-most parentheses are required.
- Inline FORTRAN keywords, **GET** and **SET**, are not allowed for defining variables.
- Parameters and optional commands within the **VAR....SUB TO....UNT** statement are explained in the following:

min i

is the lower bound for a design variable in default input units or the units specified with the **UNIT** = command. If it is not entered, the corresponding **.LE.** should also be left out.

var i

is an equipment module identifier and parameter name or stream number and property name which is to be used as design variable, e.g. **TEMPERATURE OUT** for **HEAT EXCHANGER 20**:

(**HEAT EXCHANGER (20), TEMPERATURE OUT**)  
or **FLOW** of third **COMPONENT** for **STREAM 17**:  
(**STREAM (17), FLOW COMPONENT (3)**)

max i

is the upper bound for a design variable in default input units or the units specified with the **UNIT** = command. If it is not entered, the corresponding **.LE.** should also be left out.

**UNIT** =

is the dimensional unit option associated with the design variable. It will also apply to both bounds, **TOLERANCE ABSOLUTE**, **PERTURBATION ABSOLUTE**, and the **MAXIMUM STEP** for that design variable. Optional command. If not used, the **DESIGN II** default internal dimensional unit will be used.

## **SCALE =**

is a factor which is applied to the optimization algorithm in order to alter the topology of the problem with respect to the design variable for which it is specified. The default is **SCALE = 1**.

## **TOLERANCE ABSOLUTE =**

is compared with the difference between design variables on successive iterations divided by the difference between the upper and lower bounds for the design variable. If either bound is missing the initial value of the variable is used instead. In case neither **TOLERANCE** command is specified, **TOLERANCE RELATIVE** is assumed with a default value of 0.001. Optional command.

or

## **TOLERANCE RELATIVE =**

is compared with the difference between design variables on successive iterations divided by the difference between the upper and lower bounds for the design variable. If either bound is missing the initial value of the variable is used instead. In case neither **TOLERANCE** command is specified, **TOLERANCE RELATIVE** is assumed with a default value of 0.001. Optional command.

## **PERTURBATION ABSOLUTE =**

is the adjustment of the design variable which is used to evaluate a gradient of the objective function with respect to that design variable. Units will be internal units or those specified with the **UNIT** command. Optional.

or

## **PERTURBATION RELATIVE =**

is the relative adjustment of the value for the design variable. It is multiplied by the difference between the upper and lower bounds of the design variable to determine an absolute perturbation for the design variable; if either bound is missing, it is multiplied by the initial value of the variable. In case neither **PERTURBATION** command is specified, **PERTURBATION RELATIVE** is assumed with a default value of 0.01. Optional.

## **MAXIMUM STEP =**

is the largest allowable change permitted (in default units or the units specified with the **UNIT =** command) for the search procedure from one iteration to the next. If the change according to the search vector is greater than **MAXIMUM STEP**, the search vector will be reduced (in all directions) to meet this value. Optional command. Parameters and optional commands within the **SUBJECT TO** statement are explained in the following:

## **SUBJECT TO**

is a command required only if there are any additional constraints (other than the bounds on the design variables) in the optimization problem.

## **CON(i)**

is a function of equipment parameters and/or stream properties defined by Inline FORTRAN that forms the left hand side of a constraint for the optimization. This inequality or equality expression must be satisfied for the optimization to be considered successful. For example, a constraint can be that the reboiler duty of **DIS**tillation column 17 not exceed 15 million BTU/hr. The commands for this are:

**SUBJECT TO CON(1).LE.15E6**

**F- CON(1)= GET(DIS(17),CAL DUT REB)**

Each constraint that uses the keyword **CON** must be numbered; the **CON** indicates that the constraint is defined by Inline FORTRAN statements. A maximum of 100 constraints is allowed. Simple constraints can be specified directly if the Inline FORTRAN statement does not exceed 62 characters; e.g.,

**SUBJECT TO GET(DIS(17),CAL DUT REB) .LE. 15E6**

can be substituted for the constraint definition given above.

## **constant i**

is the limiting value for the constraint. The dimensional units for this item will be internal **DESIGN II** units for equipment parameters and stream properties.

## **SCALE =**

is a factor by which the value entered as the constant is to be multiplied. The default is 1. This factor will alter the constraint and will, therefore, change the constraint. Optional command.

## **MULTIPLIER =**

is a factor by which both the constraint and the constant will be multiplied in order to emphasize or de-emphasize the constraint. Default is 1. Optional command.

**NOTE:** **SCALE** and **MULTIPLY**, if supplied, must be enclosed in parentheses immediately following the constant.

Parameters and optional commands within the **UNTIL** statement are explained in the following:

## **FUN**

is the objective function for the problem. It is an algebraic function of stream and/or equipment properties which is defined by Inline FORTRAN statements. Like **CON(i)**, **FUN** can also be specified directly, if the Inline FORTRAN statement does not exceed 66 characters.

## **SCALE =**

is a factor by which the objective function is multiplied in order to create a steeper (or shallower) response surface. The default is 1. Negative scaling factors are allowed to change the sign of the objective function. Optional command.

## Chapter 17

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### TOLerance ABSolute =

is compared to the difference between the objective function for the current optimization iteration and the previous iteration to evaluate whether an optimal solution has been reached. The objective function is in DESIGN II internal units; therefore, Inline FORTRAN expressions for FUN must be in DESIGN II internal units. Optional command.

### TOLerance RELative =

is compared to the relative difference in the objective function between the current and previous iteration. In case neither TOLerance command is specified, TOLerance RELative is assumed with a default value of 0.005. Optional command.

**NOTE:** SCA and TOL, if supplied, must be enclosed in parentheses immediately following the objective function.

### IS MINimized

indicates that the objective function is to be minimized.

or

### IS MAXimized

indicates that the objective function is to be maximized.

Two additional commands control the tolerance and set maximum iterations for the optimization run.

### OPTimization TOLerance =

is one of three criteria used to determine whether the optimization is successful. An implicitly defined non-negative function, which is derived from the Karush-Kuhn-Tucker condition, is compared to the tolerance value. The default is 0.1E-7.

### MAXimum ITERations =

is the number of iterations allowed for optimization calculations. Default is 10.

## Flowsheet Optimization Guidelines

### Flowsheet Optimization: General Discussion

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This section describes the optimization steps involved in systematically solving an optimization problem.

1. **Base case Simulation** - OPTIM first runs the base case flowsheet simulation using the values of design variables from the previous iteration (or initial guesses supplied by the user if it is the first iteration). When the base case simulation is finished the objective and constraint functions are calculated and stored.
2. **Perturbation** - OPTIM adjust (perturbs) the value of one variable by an amount which is controlled by the PER ABS or PER REL command. Then the simulation is rerun using the new value and new objective and constraint functions are calculated. If there are multiple variables, this step is repeated for each variable with all other variables at their base case values. The values of these perturbations are included in the output file.
3. **Search Vector** - OPTIM analyzes the amount of change in the objective and constraint functions with respect to each variable perturbation and determines the search vector-new values for each variable to be used in the evolutionary simulation. The new values are reported in the output file.
4. **Evolutionary Simulation** - OPTIM now performs the simulation using the new design variable values and calculates the new objective and constraint functions. OPTIM will then either start another iteration until a solution is obtained, based on the solution tolerance (discussed later), or generate a message explaining why an optimal solution was not obtained.

**NOTE:** The solution of an optimization problem often depends on the strategic use of scaling, perturbation sizes, and maximum search steps. A few case studies can provide information that leads to a choice of the variables which will reduce the overall computation time.

### Flowsheet Optimization: Basic Problem Definition

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The minimum input required to define an optimization problem and related topics are discussed below:

#### Design Variables

Design variables are defined as the stream properties or equipment parameters whose values are to be determined in order to optimize the objective function. The first design variable is preceded by the keyword VARY. Not every stream property or equipment parameter qualifies as a design variable. In the first place, it should be an item whose value can be specified in the input section (i.e. flows for specific components, total stream flow, outlet temperature for a heat exchanger, etc.). The CALculated WORK for an expander cannot be entered in the input file; consequently, it cannot be used as a design variable. A complete list of design variables for equipment modules and streams is shown in *Flowsheet Optimization: Table 1. Design variable list for OPTIM section*.

At least one design variable is required in every optimization problem. There is no limit to the number of design variables; however, computation time increases rapidly with an increase in the number of design variables.

The minimum input required to define a design variable is simply an equipment parameter or stream property as shown below.

VARY (FLAsh (20), PREssure OUT),

If the lower and upper bounds are 200 and 500 PSIA, respectively, the design variable input expands to

**VARy** (200 **.LE.** (**FLA**sh (20), **PRE**ssure **OUT**) **.LE.** 500)

Upper and lower bounds (min and max ) for each design variable are not required. Both upper or lower bound of a design variable should be provided unless it is reasonably certain that the optimum occurs at a finite value of the design variable. Otherwise, the run might terminate after the unbounded variable reaches a very large value or when the MAXimum ITERation number is exceeded

Values entered for the bounds are in the default input units or the same input units that have been defined in the GENeral section The default units can be overridden by entering the UNIt = command in the design variable statement. The specified unit should be one which is consistent with the design variable (e.g. units of degrees F, C, K, or R for any temperature specification).

**NOTE:** Liquid volume Q units (flow) are not allowed with the UNIt = command when the design variable is a stream flowrate. Initial values for design variables are provided through normal input, just as for a regular simulation run. For example,

```
*OPTIMIZE METHANE RECOVERY IN VAPOR STREAM FROM COLD SEPARATOR
VARy (200 .LE. (FLAsh (20), PREssure OUT) .LE. 500) UNTil FUN IS MINimized
F- FUN = GET(STReam (3), FLOw COMponent (2))
GENeral
COMponents = 46,2,3,4,5,6,7,8,10
FLOw 1 = 25,1000,637,475,227,300,183,215,75
TP 1 = -100,500
FLAsh 20 = COLD SEP, 1,-2,-3, PREssure OUT = 450
END
```

**NOTE:** FLO COM(2) refers to the second component in the component list, not the component ID number.

In other words, the Cold Separator (FLA 20 ) pressure of 450 PSIA serves as an initial guess rather than an absolute, unvarying input.

## Flowsheet Optimization: Constraints

Strictly speaking, simple bounds to design variables are also constraints to optimization. Constraints other than design variable bounds are entered after the keyword **SUB**ject **TO** and before the keyword **UNTil**, using **CON**straint phrases arranged in any order. The minimum input for a constraint is

```
.LE
or
CON(i) .EQ constant
or
.GE
F- CON (i) = GET(....)
```

CON(i) can also be explicitly defined by an Inline FORTRAN statements, e.g.,

```
GET (....) .LE. constant
```

Both constraints and objective function can be entered as Inline FORTRAN statements beginning with **F-** or they can be defined with Inline FORTRAN expressions explicitly. Both implicit and explicit statements can be used in the same run. Each **CON**straint which is entered using the keyword **CON** (i.e. not defined explicitly) must be numbered between 1 and 100. There is no requirement that the numbers be in ascending or sequential order. The maximum number of constraints (implicit and explicitly defined) is 100. The number of independent equality constraints cannot exceed the number of design variables.

```
GET(STR (3),FLO COM(1)) + GET(STR (3),FLO COM (2)) .LE. 100
```

Constraints are evaluated using the **DESIGN II** internal units set. The numerical value for the constant should also be in internal units. Briefly, the internal units set is

temperature	degrees R
pressure	PSIA
quantity	lbmoles
heat, energy	BTU
length	feet
time	hours

A complete list of dimensional units associated with equipment and stream parameters can be found in *Inline Fortran: Table 2. Flowsheet Parameters Available to GET and SET*, of the Inline FORTRAN section.

The constant for the constraint can be scaled by a factor which is entered with the **SCA**le command. Effects of scaling will be discussed in more detail later, as will **MUL**tiplication.

## Flowsheet Optimization: Objective Function

Every optimization problem is required to have an objective function. The objective function is a function of equipment parameters or stream properties that is to be made as small (**MIN**imized) or as large (**MAX**imized) as possible. The objective function begins with the keyword **UNTil** using **FUN**ction or an explicit Inline FORTRAN statement. For example, the

## Chapter 17

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horsepower from expander numbered 37 in the flowsheet input could be maximized with the statements

```
UNTil FUN IS MAXimized
F-      FUN = GET (EXPander (37), CAL WOR)
```

or equivalently:

```
UNTil GET(EXPander (37), CAL WOR) IS MAXimized
```

In general, the list of equipment parameters and stream properties shown in *Inline Fortran: Table 2. Flowsheet Parameters Available to GET and SET*, in the Inline FORTRAN section is available for use as constraints and objective function values. *Flowsheet Optimization: Table 1. Design Variable list for OPTIM Section* of this section is the subset of that list which can be used as design variables

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### Flowsheet Optimization: Solution Tolerances

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The solution tolerance will be the default tolerance unless it is changed by using one or more of the tolerance commands. The optimization calculation continues to iterate until it attains an optimal solution as defined by any one of the following occurrences:

1. A consecutive iteration fails to improve the objective function by more than a given tolerance, on condition that all the constraints (including variable bounds) are reasonably met. Objective function tolerance is specified using the TOLerance ABSolute or TOLerance RELative command which follows the keyword FUN (or its explicit definition). If only TOLerance is entered, it is assumed to be TOLerance ABSolute. For TOLerance RELative, the tolerance is applied to the prevailing value of the objective function. The default is a relative tolerance of 0.005.
2. The change in every design variable for consecutive iterations is less than a given tolerance. Design variable tolerances are specified using the TOLerance ABSolute or TOLerance RELative command following the definition of variables. If only TOLerance is entered, it is assumed to be TOLerance ABSolute. Tolerances may be specified as ABSolute values for some variables, and as RELative values for others. For the RELative option, the tolerance applies to the specified range of the design variable, which is defined as the difference of the corresponding upper bound and lower bound. If either bound is missing, the tolerance applies to the initial guess for that variable. The default is a relative tolerance of 0.001 for every variable.
3. An implicitly defined non-negative function becomes smaller than the OPTimization TOLerance. This function is derived from the Karush-Kuhn-Tucker conditions. The default value for OPTimization TOLerance is 10<sup>-8</sup>. Normally, this command will not be needed.

DESIGN II execution will also terminate when better designs cannot be located along the search vector, even if none of the above criteria are satisfied. In this case, a decision must be made about whether the solution at the last iteration is satisfactory. If it is not, another set of initial guesses and/or algorithmic parameters must be tried (see *Flowsheet Optimization: Scaling*, *Flowsheet Optimization: Perturbation Size* and *Flowsheet Optimization: Maximum Search Step*).

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### Flowsheet Optimization: Scaling

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Proper scaling is important in achieving good optimization results. Design variables, constraints and the objective function each have a SCAle command. A MULTiply command is also available for constraints. The effect of scaling is different for each.

Scaling of design variables changes neither the problem nor the true solution. It does, however, alter the topology of the problem. Essentially, larger scaling factors yield steeper gradients of objective function with respect to the corresponding variables. The default SCAle factor for design variables is 1.0.

The objective function can also be scaled. Here, the objective function is actually changed but the true solution of the design variables remains the same if the scaling factor is positive. A higher objective scaling factor gives a steeper response surface in all directions.

Constraints can be scaled by factors you enter with MULTiply commands. Both sides of the constraint expression will be multiplied by these factors. Constraint multiplication does not change the true solution. It is used to emphasize or de-emphasize individual constraints, especially when equality (.EQ.) constraints are involved. Note the difference between MUL factors and SCAle factors for constraints: the SCAle factor only applies to the value entered as a constant and will very likely to change the true optimum. The MULTiply command can be used to ensure that the constraint value(s) will be the same order of magnitude as the objective function value.

**NOTE:** Only the objective function can have a negative scale factor.

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### Flowsheet Optimization: Perturbation Size

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Perturbation sizes for design variables can be specified using the PERTurbation ABSolute or PERTurbation RELative phrase, following the same convention as for design variable tolerances. The default is a relative tolerance of 0.01 for each variable. The perturbation size must be sufficiently large to cause a measurable change in the objective function. If it is too small, the optimization algorithm will be ineffective in performing the search procedure. While the default perturbation should be suitable for many variables, a knowledge of the flowsheet may be a guide to providing a better value.



## Flowsheet Optimization: Maximum Search Step

Maximum search steps of design variables can be specified using the MAXimum STEp command. Normally this command is not needed. By default, a search vector is determined by the optimization routine and implemented as such. However, if MAXimum STEp has been specified and the next step calculated by the optimization algorithm exceeds this maximum step, the search vector will be reduced in all directions.

## Flowsheet Optimization Reference Tables

A list of equipment parameters and stream properties which may be used as design variables for optimization is shown below. Those listed are a subset of all variables available to Inline FORTRAN. The Inline FORTRAN convention of equipment module identifier, equipment number, and equipment parameter keyword (including index, if the parameter can have multiple values) must be followed, i.e. (module identifier(equipment number), parameter keyword (index position)). For example, the outlet pressure of PREssure OUT for COMpressor 35 would be defined as

(COMPRESSor(35), PREssure OUT)

The left most and right most parentheses are required. The Inline FORTRAN keywords, GET and SET, are not allowed for defining design variables.

### Flowsheet Optimization: Table 1. Design Variable list for OPTIM Section

#### Flowsheet Optimization: COMponent SPLitter Options

<b>REC TOP (i)</b>	Recovery of a component (position order) in the top product (fraction or flowrate as specified in COMponent SPLitter)	<b>TEM BOT</b>	Bottom product temperature specification
		<b>TEM TOP</b>	Top product temperature specification

#### Flowsheet Optimization: COMPRESSor Options

<b>EFF</b>	Efficiency	<b>TEM BUB</b>	Temperature specification for bubble point pressure calculation
<b>POL COE</b>	Polytropic coefficient	<b>TEM DEW</b>	Temperature specification for dew point pressure calculation
<b>PRE OUT</b>	Final discharge pressure	<b>TEM INT</b>	Interstage cooler temperature; one value for all stages
<b>PRE STA (i)</b>	Discharge pressure for stage i, maximum stages = 10	<b>WOR AVA</b>	Horsepower available for compression
<b>STE IN</b>	Driver inlet steam enthalpy		
<b>STE OUT</b>	Driver outlet steam enthalpy		

#### Flowsheet Optimization: DISTillation Column Options

<b>DEC REF</b>	Solubility of immiscible component in reflux (mole fraction)	<b>REB</b>	Reboiler duty
<b>DEL</b>	Pressure drop through column	<b>REF</b>	Reflux ratio
<b>DUT CON</b>	Condenser duty	<b>TEM CHI</b>	Chiller temperature for pre-saturator option
<b>HEA (i)</b>	Heat added to or removed from (negative value) a tray in top to bottom order	<b>TEM CON</b>	Condenser temperature
<b>PRE CON</b>	Condenser pressure	<b>TEM CON SUB</b>	Degrees of subcooling for condenser (TOT, STR TOT)
<b>PRE TOP</b>	Top tray pressure	<b>TEM INT (i)</b>	Intercooler return temperature for "ith" intercooler
<b>PRO (i)</b>	Product rate from column in top-to-bottom order (fractional or molar rate as specified in DIS)	<b>TEM REB</b>	Reboiler outlet temperature
		<b>THE</b>	Mole fraction of vaporization from reboiler

#### Flowsheet Optimization: DIVider Options

<b>FLO RAT (i)</b>	Fraction or flowrate for the "ith" outlet stream as specified in DIVider
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#### Flowsheet Optimization: EQUilibrium REActor Options

<b>EXT (i)</b>	Extent of reaction "i"; reaction "i" must be defined
<b>TEM REA (i)</b>	Temperature approach for reaction "i".

#### Flowsheet Optimization: EXPander Options

<b>EFF</b>	Adiabatic efficiency for expander (isentropic)
<b>PRE OUT</b>	Final discharge pressure

#### Flowsheet Optimization: FIRed Heater Options

<b>DEL</b>	Pressure drop through heater	<b>RAT HEA</b>	Rating of heater
<b>EFF</b>	Fuel efficiency	<b>TEM OUT</b>	Process stream outlet temperature
<b>HEA VAL FUE</b>	Heating value for fuel		

#### Flowsheet Optimization: FLASh Options

<b>HEA</b>	Heat added to or subtracted from (negative	<b>PRE OUT</b>	Discharge pressure for outlet stream(s)
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## Chapter 17

<b>LIQ FRA</b>	value) the inlet stream Specified liquid fraction for flash	<b>TEM OUT</b>	Outlet temperature for product stream(s)
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### Flowsheet Optimization: HEAt EXChanger Options

<b>ARE</b>	Area per shell for exchanger	<b>TEM APP</b>	Approach temperature between second inlet and first outlet stream
<b>DEL (i)</b>	Pressure drop for shellside, tubeside streams	<b>TEM OUT</b>	Outlet temperature for first product stream
<b>DEL TEM</b>	Outlet temperature of first stream - inlet temperature of first stream	<b>TEM REF</b>	Temperature for the refrigerant, P calculated
<b>DUT</b>	Specified duty	<b>TEM WAT IN</b>	Cooling water inlet temperature
<b>PRE REF</b>	Pressure for the refrigerant stream, T calculated	<b>TEM WAT OUT</b>	Cooling water outlet temperature
		<b>U</b>	Overall heat transfer coefficient

### Flowsheet Optimization: HYdroTReater Options

<b>ARO CON</b>	Mole fraction of aromatics in feed stream	<b>PRE DRO</b>	Pressure drop per bed
<b>ARO REA</b>	Mole fraction converted to saturated hydrocarbons	<b>PRE QUE</b>	Quench stream pressure
<b>NIT CON</b>	Weight fraction of nitrogen in feed stream	<b>SUL CON</b>	Weight fraction of sulfur in the feed stream
<b>NIT REA</b>	Weight fraction of nitrogen converted to ammonia	<b>SUL REA</b>	Weight fraction of sulfur converted to hydrogen sulfide
<b>OLE CON</b>	Mole fraction of olefins in feed steam	<b>TEM DRO (i)</b>	Temperature drop for bed "i"
<b>OLE REA</b>	Mole fraction of olefins converted to saturated hydrocarbons	<b>TEM QUE</b>	Temperature of the quench stream
		<b>TEM RIS (i)</b>	Temperature rise for bed "i"

### Flowsheet Optimization: LNG Exchanger Options

<b>ARE (i)</b>	Area per shell "i"	<b>TEM APP (i)</b>	Tube side outlet stream "i" temperature - shellside inlet stream temperature
<b>DEL TUB (i)</b>	Pressure drop for tube stream "i"	<b>TEM OUT (i)</b>	Outlet temperature of tubeside stream "i"
<b>DEL SHE (i)</b>	Pressure drop for shell stream "i"	<b>U (i)</b>	Heat transfer coefficient for tubeside stream "i"
<b>DUTY (i)</b>	Heat added to or removed from (negative value) tubeside stream "i"		

### Flowsheet Optimization: POLytropic Compressor Options

<b>SPE</b>	Radial speed
<b>THE FAC</b>	Thermodynamic factor

### Flowsheet Optimization: PUMp Options

<b>EFF</b>	Efficiency	<b>WOR AVA</b>	Horsepower available for pumping
<b>PRE OUT</b>	Final discharge pressure		

### Flowsheet Optimization: SHORtcut Fractionator Options

<b>DEL</b>	Pressure drop through column	<b>REC BOT</b>	Mole fraction of heavy component in bottom/heavy key in feed
<b>PER MIN</b>	Percent of minimum reflux ratio	<b>REC TOP</b>	Mole fraction of light component in overhead/light key in feed
<b>PRE TOP</b>	Top product pressure		

### Flowsheet Optimization: STReam MANipulator Options

<b>FAC (i)</b>	Factor by which the component flowrate in the "ith" position in COMponent list will be ADDED, SUBtracted, MULtiplied or DIVided
----------------	---------------------------------------------------------------------------------------------------------------------------------

### Flowsheet Optimization: STReam Properties Options

<b>FLO COM (i)</b>	Flowrate of component "i", position order in COMponent list	<b>PRE</b>	Pressure of the stream
<b>FLO</b>	Total flow for stream	<b>TEM</b>	Temperature of the stream

### Flowsheet Optimization: VALve Options

<b>DEL</b>	Pressure drop across valve
<b>PRE OUT</b>	Outlet pressure
<b>TEM BUB</b>	Temperature specification for bubble point calculation
<b>TEM DEW</b>	Temperature specification for dew point calculation

## Flowsheet Optimization: Table 2. DESIGN II Utilities Available in OPTIM Section

Inline FORTRAN also provides certain utility subroutines that may be used in defining constraints and objective function. Only the names and a brief description of each will be shown here. For a complete list and more detailed information on structure and usage, please refer to Tables 2, 3, 5, 6 and 7 in Inline FORTRAN Section.

### 1. General (use with **CALL**)

<b>COPSTR (i, j)</b>	Copies all information about stream "i" into stream "j".
<b>INISTR (i)</b>	Use to initialize stream "i" after changing parameters with SET.
<b>RAPSON</b>	Solves set of nonlinear equations.
<b>KVALUE</b>	Calculates K-values for a stream.
<b>VAPENT</b>	Calculates vapor enthalpy for a stream.
<b>LIQENT</b>	Calculates liquid enthalpy for a stream.
<b>DENSTY</b>	Calculates densities for a stream.
<b>THRCON</b>	Calculates vapor or liquid thermal conductivity.
<b>VISCOS</b>	Calculates vapor or liquid viscosity.
<b>SURTEN</b>	Calculates surface tension for a liquid stream.

### 2. Component Point Properties (use with **GET(BANK(xxx),POS(yyy))**)

<b>ATC, APC, AVC</b>	Critical point values; T, P, and V
<b>API, SPGR, GPMP (60 F, 14.696PSIA)</b>	API gravity, specific gravity, gallons/lbmole
<b>ATB, AMW</b>	Normal boiling point, molecular weight
<b>ADEL, AOMA, WATK, AVW</b>	Solubility parameter, acentric factor, Watson K factor, characteristic volume
<b>IDCO, KOMN (i)</b>	Component id. number, component name

## Flowsheet Optimization Examples

There are several sample flowsheets in "Chapter 51: Optimization Samples - c:\designii\samples\optimize" of the DESIGN II for Windows Tutorial and Samples Guide.

## Flowsheet Optimization Reference

1. "Engineering Optimization - Methods and Applications", G.V. Reklaitis, A. Ravindran, and K.M. Ragsdell, John Wiley and Sons, New York, 1983.



# Chapter 18: Inline FORTRAN

## Inline FORTRAN Overview

Inline FORTRAN enables integration of FORTRAN 66 commands directly into a DESIGN II input file. Custom tailored process simulations that meet exact requirements can now be developed by:

- Modifying the existing DESIGN II equipment module calculations (GET/SET)
- Developing subroutines, subroutine libraries and creating your own equipment modules
- Accessing DESIGN II internal subroutines and functions

DESIGN II makes these operations easy to implement by using simple keyword phrases. All FORTRAN statements are compiled during run time by the DESIGN II internal compiler, immediately after the DESIGN II input data has been processed. Then the code is linked to the DESIGN II program to form an executable "module".

## Inline Fortran Command Details

This section is organized according to the three typical uses of Inline FORTRAN described in the "Overview" section. However, there are several commands that are common to all three uses. These commands are described below.

### DEBUG LIMIT

Add this command to a set of Inline FORTRAN commands either in an equipment or in a subroutine. Indices on subscripted variables will automatically be compared with the dimensions on that variable in a DIMENSION statement. If the limits of the DIMENSION statement are exceeded, an error message will be generated. This is an important tool for automatic checking of Inline FORTRAN code.

Inline FORTRAN code can be filed and saved. This makes it easier to use the same Inline FORTRAN in different DESIGN II input files. Three commands exist for manipulating Inline FORTRAN files. For all three commands, the file name consists of three separate entries (name1, name2, name3) separated by commas and each four characters long beginning with an alphanumeric character.

### NEW FORtran FILE = name1, name2, name3

Causes a file to be created and saved containing the current compiled Inline FORTRAN.

### OLD FORtran FILE = name1, name2, name3

Causes the compiled routines on an existing file to be used in addition to new Inline FORTRAN for linking. To save the new code (if input file contains FORTRAN changes) append ,3 after the last file name, E.g. OLD FOR FIL = NAM1,NAM2,NAM3,3.

### ERASE FORtran FILE = name1, name2, name3

Causes an existing Inline FORTRAN file to be deleted

---

## Inline Fortran: Existing Equipment Module Modifications

---

DESIGN II provides for the entry of FORTRAN statements directly in equipment module sections. These statements can be used to perform operations on practically any parameter or values associated with a flowsheet simulation. In particular, equipment and stream parameters can be obtained from the internal storage areas of DESIGN II and stored back into these areas with FORTRAN statements. Almost any legal FORTRAN operation can be performed with these parameters, including algebraic statements, loops, conditional jumps, etc. All of these statements can be placed directly in the equipment module. The few exceptions or differences from FORTRAN 66 are listed in *Inline Fortran: Table 1. Inline FORTRAN Restrictions*.

### Entering FORTRAN Statements

To use the flowsheet parameter phrases in FORTRAN statements, first identify any FORTRAN commands to DESIGN II. This is done by beginning each FORTRAN line with F-. The FORTRAN coding then follows, using the normal formatting.

Note that the FORTRAN statement actually begins in column 9 rather than column 7 since F- occupies columns 1 and 2.

### GETting and SETting Flowsheet Parameters

The functions required to obtain (GET) a flowsheet parameter value and to store (SET) a new value are:

equipment id -->1

**GET**( or (number) , parameter name (position) )  
STReam

and

equipment id -->1

**SET**( or (number) , parameter name (position) )

## Chapter 18

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### STream

The equipment module id is the usual DESIGN II equipment module identifier, (spelled out in full or abbreviated); such as,

**PUM** for a pump

**DIS** for a distillation module

**COMPRE** for a compressor

The number following the module identifier is the number of the equipment in the flowsheet.

The parameter names are the standard keyword phrases which are used for equipment and streams described in the appropriate sections of the DESIGN II User's Guide. A complete list of flowsheet parameters which can be accessed by GET and SET are included in Tables 2 and 3 at the end of this section. Both Tables also list the internal dimensional units for each retrieved flowsheet parameter. Any values to be stored into DESIGN II must be converted to internal units to be consistent.

Here are some examples GET and SET phrases:

```
SET (COMPRE(2), PREOUT) = 1000
```

Changes the specified outlet pressure for Compressor 2.

```
T1 = GET (STR(14), TEM)
```

Retrieves the temperature of Stream 14 for use in a subsequent calculation.

```
HSID3 = GET (DIS(2), HEA(3))
```

Retrieves the duty for heater/cooler 3 of DISTillation column 2.

```
SET (HEA EXC(7), DUT) = 1.5E6
```

Changes a specified duty for Heat Exchanger 7.

The following examples show some valid FORTRAN statements using the GET and SET phrases. Using a compressor described in a flowsheet as:

```
COMPRE 23=GAS,32,-33, PREOUT=800
```

the work required for the compression could be retrieved and stored as a FORTRAN variable "WORK" for use in subsequent statements. The command for retrieving the required work for COMPRE 23 is simply:

```
F- WORK=GET (COMPRE (23), CALWOR)
```

A calculation requiring some logic can also be performed. For example,

```
F- WORK = .95*GET (COMPRE (23), CAL WOR)
```

or

```
F- IF (GET (COMPRE (23), CAL WOR) .GT. 1.E04) WORK = 1.E04
```

Additionally, a new outlet pressure for Compressor 23 can be stored for subsequent calculations:

```
F- (WORK/GET (COMPRE (23), CAL WOR)) *
```

```
F- GET (COMPRE (23), PREOUT)
```

```
F- SET (COMPRE (23), PREOUT) = POUT
```

Frequently, DESIGN II input commands require the entry of more than one item on the right hand side of the equals sign. For example, for a multistage compressor,

```
PRE STA = 125, 325, 800
```

The GET and SET functions can process only one item at a time. Consequently a "position" or index is required to indicate which item is being retrieved (with GET) or stored (with SET). For example, the following commands would increment the pressure of the stages by 5 PSIA on each loop of a recycle:

```
COMPRESSOR 23 = GAS, 32, -33, PRESSURE OUT = 800
```

```
ENTROPY, EFFICIENCY = .72
```

```
STAGES = 3, PRESSURE OF STAGES = 125, 325, 800,
```

```
TEMPERATURE OF INTERCOOLERS = 100
```

```
F- DO 100 J = 1, 3
```

```
F- PRESS = GET (COMPRE (23), PRE STA (J))
```

```
F- SET (COMPRE (23), PRE STA (J)) = PRESS + 5.
```

```
F- 100 CONTINUE
```

```
F- SET (COMPRE (23), PRE OUT = GET (COMPRE (23), PRE STA (3))
```

Note the following rules for using the GET and SET functions:

- The SET function is a nonstandard FORTRAN function and can only be used on the left hand side of an equals sign to store a value for a flowsheet parameter.
- The SET function may not be used to store calculated parameters such as the ones below. Only use the GET function when referring to these calculated parameters.

**CAL**culated **WORK**

**CAL**culated **ELE**ctrical power usage

**CAL**culated **FUE**l gas consumption

**CAL**culated **STE**am consumption

**CAL**culated **WATE**r for cooling

**CAL**culated value per **MOL**

**CAL**culated value per **SCF**

- Both functions are nonstandard in that their arguments are character strings instead of the usual one to six character name used for FORTRAN variables. For example, the command

**GET(COMPRES (23), CALWOR )**

can be written in the expanded version shown below for clarification:

**GET(COMPRESSOR(23), CALCULATED WORK)**

- DESIGN II streams are always at equilibrium for the given temperature and pressure. When a stream parameter is adjusted by using the SET function, the stream information may no longer reflect an equilibrium mixture. In some cases this may be the desired result, but in most cases the library function

**INISTR (i)**

- must be used to reinitialize stream "i" so that the vapor and liquid compositions will reflect an equilibrium mixture. See *Inline Fortran: Table 6. Thermodynamic Library Subroutines* for an explanation of this library function.

### Controlling When FORTRAN Is Executed

FORTTRAN statements may be located on any line of an equipment module section after the topology definition. FORTRAN statements for an equipment module are executed before the module itself is calculated unless indicated otherwise. You can explicitly state when the FORTRAN is executed with the PRE, POST and DURING statements described below:

Command	Result
F- PRE	process FORTRAN statements before equipment calculation
F- POST	process FORTRAN statements after equipment calculation
F- DURING	process FORTRAN statements during equipment calculations. Only available for rigorous DISTillation, PLUG flow REactor, and CSTR.

**NOTE:** 6 blank spaces must separate "F-" and PRE, POST or DURING

The following rules must be followed when using the PRE, POST, and DURING statements:

- The PRE, POST, or DURING statements must be the first of the Inline FORTRAN statements within an equipment module.
- Only one of these statements per module can be specified
- To execute the same FORTRAN statements before and after an equipment calculation (e.g. for comparison purposes), add the same FORTRAN statements to two consecutively calculated equipment modules with PRE specified for the first equipment module and PRE specified for the second.
- For the DISTillation column, the results for product streams leaving the module will not be written until calculations are completed. With the "DURING" command, intermediate results can be accessed or displayed with FLOWL or FLOWV. See *Inline Fortran Table 3. DISTillation Function*, in this section. A requirement for DURING operations in DISTillation is that you **must** define an EPS(1) specification, which will replace a PURity, RATio or RECOVERY specification (see Example 2). If you define both EPS(1) and EPS(2), you must have entered two composition specifications in your input.

### Writing Results to the Printout And Displaying Results On The Screen

To record the results of FORTRAN calculation in the printout file, the standard FORTRAN statements, WRITE and PRINT, are available. All output, for both PRINT and WRITE, will occur after the "NOW CALLING" heading for the appropriate equipment in the DESIGN II output (PRE processed FORTRAN will appear before the specific module in the equipment's "NOW CALLING" heading).

The PRINT statement does not require a FORMAT statement and is written:

F- PRINT argument

where "argument" can be a scalar or an element of an array (names are limited to a maximum of 6 characters).

The WRITE statement syntax is:

F- WRITE (6,XXX) var

where 6 indicates the regular output file, XXX is the number of the accompanying FORMAT statement, and "var" can be one variable name or a list of variable names separated by commas whose values are to be written. Inline FORTRAN also has the capability to direct results of queries to the terminal screen for interactive processing. (This feature is available only for computers on which DESIGN II can be executed interactively, not for batch execution.) The "WRITE(1,XXX) var" statement will write the value of the specified variable to the terminal screen (1 = screen). The "READ (1,XXX)var" statement will read a value entered on the terminal screen and store the value under the specified variable name. In order to simplify the FORTRAN statements required to READ from and WRITE to the screen, Inline FORTRAN includes the commands: INPUT and DISPLAY.

The input command syntax is

var = INPUT (PROMPT CHARACTER STRING)

where "var" is the variable name into which the number entered on the screen is to be stored and "prompt" is the message to be written to the screen to prompt the user to enter the number. The equivalent standard FORTRAN statements required for the same result are

## Chapter 18

---

```
      WRITE (1,XXX) var
XXX   FORMAT (1X,'prompt')
      READ (1,XXX) var
XXX   FORMAT (....)
```

The DISPLAY command syntax is

```
DISPLAY (PROMPT CHARACTER STRING) var
```

where "prompt" is the message to be printed in front of the variable value to be written and "var" is the name of the variable value to be written. The equivalent standard FORTRAN statements required for the same result are:

```
      WRITE (1,XXX) var
XXX   FORMAT (1X,'prompt',1PG15.5)
```

The DISPLAY and INPUT commands make creating an interactive program a simple task. Mathematical operations in the arguments of these two commands are not allowed.

**NOTE:** DISPLAY and INPUT commands in Inline FORTRAN cannot handle the following:

1. Lower case characters
2. Arithmetic operations

### Character Data

Inline FORTRAN can read character data using the Hollerith data format

**Example:**

```
INTEGER ITEXT (10)
INTEGER ITEXT (40)
DATA ITEXT/4 HINLI, 4HNE F, 4HORTR, 4HAN M,4HAKES,4HDES,
*4HIGN,4HII U,4HNIQU,4HE /
WRITE(6,100) (ITEXT(I),I-1,10)
100 FORMAT (X,10A4)
```

**Results:** INLINE FORTRAN MAKES DESIGN II UNIQUE

---

## Inline Fortran: User Added Equipment Modules ADD Blocks

---

ADD blocks are user written FORTRAN models of equipment which can be added to DESIGN II. These blocks are usually highly specialized equipment models but can also be used to perform general operations on stream and equipment variables. This capability to add user-written FORTRAN equipment models has been present in DESIGN II for a number of years, but required that the operations of compilation and linking be performed externally to DESIGN II. Inline FORTRAN now eliminates the need to perform the compilation and linking steps to add a ADD block routine to DESIGN II. With this method the ADD block routines can be entered in the DESIGN II input file along with standard equipment modules. Compilation and linkage steps, now internal to DESIGN II, are automatic.

The following DESIGN II keywords are required to be defined in the equipment module section of the input file. All commands are required:

**ADD** i = name, streams

This is the ADD block module command, where "i" is the assigned flowsheet equipment number, name is the equipment name, up to 16-characters, and streams are the inlet and outlet stream(s) numbers.

Alternatively, using the graphical user flowsheet the user can select a generic module (1 or 2) and use Keyword Input to select ADD module and start with the following Keyword Commands

**USE BLOCK** j

This keyword designates which BLOCK of subroutines from the FORTRAN library section will be used to execute the ADD module, where "j" is the BLOCK number.

**NEQ**p = k

This is the number of equipment parameters that will be input and/or generated during the ADD block subroutine calculations. The ADD block module number "i" must also be included in this count.

**EQP**ar list = values

This is a list of values to be used in the ADD block calculations as well as any values that are calculated within the ADD block which you want to save. The calculated results may then be passed on as input to other DESIGN II equipment modules or subroutines. Accessing equipment parameters for use in subroutines is explained further in the *Add Module: Essential Data Interface Within ADD Blocks* section.

The following command is required after the FORTRAN keyword but before STArT LIBRARY in the input file or under Specify...Inline Fortran section in the Main Menu of the graphical user interface.

**BLOCK** j = number of subroutines, subroutine names

The BLOCK command must appear between the FORTRAN command and the STArT LIBRARY command in the FORTRAN library section. "j" is the BLOCK number assigned in the USE BLOCK command. Number of subroutines is the total number of subroutines in the following list of subroutines to be called. The first name listed is the main subroutine of the ADD BLOCK and is executed first. The other subroutines listed are those called by the first subroutine. The FORTRAN library must be the last



section of the input file.

## Function Of Add Blocks

The order of calculation of ADD blocks in a flowsheet is governed by the same rules for calculation sequences as other unit operation modules. The function of the ADD block is to calculate the output stream conditions from the input stream conditions and to perform any other calculations the user has defined.

The order of calculations in an ADD block is:

1. Access all input stream information from DESIGN II.
2. Perform the heat and material balance calculations (or whatever calculations the user has defined).
3. Flash all output streams with FLASH1 (see Table 8).
4. Return all output stream information to DESIGN II.

## Inline Fortran: Subroutines for both Existing Equipment Modifications and ADD Blocks

The Inline FORTRAN feature also allows creation of subroutines (i.e., a set of FORTRAN calculations that can be performed repeatedly within a program). This is accomplished in DESIGN II by adding a new input section which begins with the keyword command, FORTRAN.

The FORTRAN library is considered similar to other modules which perform specific functions; e.g., DIS for distillation, FLA for flash calculations, and GENERAL for entry of stream information, thermophysical property options, units options, etc. After the FORTRAN keyword, the subroutines are entered. One of several subroutines may be entered within the FORTRAN module.

There are three keyword commands within the FORTRAN module: STArt LIBrary, STOP LIBrary and BLOck j = *list*. STArt LIBrary and STOP LIBrary are always required when using the FORTRAN module.

### STArt LIBrary

Indicates that all the commands which follow are to be treated as standard FORTRAN; that is, columns 1-5 are for statement numbers, column 6 is for a continuation of the previous line, and columns 7-72 for FORTRAN statements. A "C" in column 1 indicates a comment statement.

### STOp LIBrary

indicates the end of the FORTRAN statements.

### BLOck j = *list*

The BLOck command is used when user-created equipment modules are included in the simulation. This command is described previously in the ADD block section.

Two other commands, INCLUDE and CALL are required in the equipment module to access the subroutines:

### INCLUde namex, namey,...

This command is required to access a subroutine from the FORTRAN library for use in an equipment module, where NAME is the subroutine name(s) to be called. This command must be included in the Inline FORTRAN before the traditional CALL statement, and located within the same equipment module as the CALL statement.

### CALL namex

The traditional CALL statement for accessing subroutines.

The following example shows a skeleton structure of a DESIGN II program which includes FORTRAN subroutines.

```
*DUMMY OUTLINE OF SUBROUTINE USAGE HEA EXC 1 = ...
FLA 2 = ...
PUM 5 = ...
HEA EXC 10 = ...
F-      POST
F-      INCLUDE CASES
F-      COMMON/SAVEBK/ICASE, DUMMY (4, 40)
F-      .
F-      .
F-      .
F-      CALL CASES (TEMP, PRES, WORK, BOILER)
F-      .
F-      .
F-      .
GENERAL,
      .
      .
      .
FORTRAN
START LIBRARY
SUBROUTINE CASES (T, P, W, B) COMMON/SAVEBK/ICASE, TS (40), PS (40), WS (40), BS (40)
      TS (ICASE) = T
      .
      .
      .
      100      WRITE (1, 300)
      300      FORMAT (...)
```

```
RETURN
END
STOP LIBRARY
END
```

**NOTE:** Common blocks can be used in Inline FORTRAN for the same purposes as in standard FORTRAN-to communicate variables from one subroutine to another and, for DESIGN II, to communicate variables from one equipment module to another. They can also be used to initialize variables to zero, since all common block variables are set to zero before execution.

## Inline Fortran Guidelines

The DESIGN II simulation program offers a wealth of equipment module and stream property calculations, equipment sizing and rating, and full flowsheeting capabilities, such as handling recycle convergence, optimization, and case studies. With Inline FORTRAN, you have the power to extend calculations even further. You can define your own proprietary reaction calculations, create your own Distillation product composition specifications, define additional stream property calculations or special reports and much more. All compilation and linkage is handled automatically by DESIGN II (FORTRAN 66). Simply follow 6 easy steps. Each step will be discussed in detail below.

1. Determine the proper placement of your Inline FORTRAN statements:

*in DESIGN II equipment module sections,  
in user-defined equipment modules (ADD Block),  
in a FORTRAN Library,  
in all 3 locations in the same simulation*

2. Choose from the DESIGN II equipment and stream specifications or calculations and physical property and thermodynamic routines available to be used to perform additional calculations or create reports (see Tables 2 -9).
3. Prepare equations, if any. Standard arithmetic functions are supported (+, -, \*, /, \*\*), as well as a RAPHSON convergence algorithm.
4. *Add Inline FORTRAN statements* to your input file using a combination of keywords and regular FORTRAN coding statements.
5. *Add optional FORTRAN commands.*
6. *Inline Fortran: Review FORTRAN Coding* - Check your coding and review the Inline FORTRAN restrictions.

---

## In DESIGN II Equipment Module Sections

---

DESIGN II allows you to use equipment specifications, calculated equipment parameters, most stream properties, and pure component physical properties in the FORTRAN statements you define. FORTRAN commands can be placed directly in one or more equipment module keyword sections. See example *Inline FORTRAN: Gas Plant Feed Chillover*.

These FORTRAN calculations can take place before, after, or during the calculations of the equipment module where the Inline FORTRAN commands were placed.

- F- **PRE** before module calculations (default)
- F- **POST** after the equipment calculation
- F- **DURING** while equipment calculations are being performed (DISTillation, CSTR and PLUG flow REactor only)

SIX special operations are available, in addition to regular FORTRAN statements you provide.

**GET** Retrieve a stream property or equipment parameter

**SET** Change an equipment specification, stream property, or Design II property bank value (syntax for property bank usage can be found in Tables 5 and 8)

**DISPLAY**(text label) variable

Write a value to the computer screen (using INTeractive option) variable=INPUT(Prompt character string). Read a value the user enters from the keyboard (INTeractive option)

**PRINT** variable

Write a value to the output file (in the NOW CALLING section for the equipment module(s) where the FORTRAN commands are placed)

**INCLUDE** namex, namey

Specify the name(s) of subroutines in the FORTRAN LIBRARY to be used in equipment module Inline FORTRAN, if any regular FORTRAN READ and WRITE commands are available also. Details on the syntax for INPUT, PRINT

and DISPLAY can be found in *Inline Fortran: Command Details*.

## Chapter 18

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### In user-defined equipment modules (ADD block)

---

You can create an ADD block which performs a set of calculations which you define, such as a proprietary unit operation, economics calculations, complex heat transfer or pressure drop calculations or define special reports. The ADD block will use 1 or more FORTRAN subroutines which will be defined in a FORTRAN LIBRARY. ADD blocks share many of the features of other equipment modules:

1. an equipment module identifier (ADD)
2. a unique equipment number
3. a flowsheet name of up to 16 characters
4. inlet and outlet streams(s)

See ADD Block Command Details to follow *Procedures For Writing ADD Modules* within DESIGN II and the details on the usage of these commands. The *Add Module: Essential Data Interface within ADD Blocks* section also explains the subroutine arguments which are automatically available to ADD Blocks for communication of data to and from the DESIGN II data structures.

An essentially unlimited number of inlet streams may be connected to the ADD block; they will be adiabatically mixed and flashed to the lowest stream's pressure. Phase separation results can be stored in the first three outlet streams (if provided). The number of inlet or outlet streams may be limited in the ADD block definition. Notify the ADD block users of any restrictions on number of inlet or outlet streams.

The next few commands are unique to ADD blocks.

USE BLOCK j

Indicates the set of subroutines to be used for the ADD block; j is the Block number in the FORTRAN Library.

NEQp =

Total number of input values and calculated values to be used/reported by the ADD Block.

EQPAR=value, value, value....

Values for input parameters, separated by commas; calculated values will be added on completion of ADD Block calculations.

The NEQ keyword stands for "number of equipment parameters" and includes all the values which will be entered as input as well as the values you want reported in the Equipment Summary section of the output. The first position in the EQPAR list (EQUIPMENT PARAMETERS) must be reserved for the equipment module number. Be sure to include it in your count.

The second position of the EQPAR list serves a dual purpose. You can store an input (or calculated) value there. It is also the position used to determine which type of flash to perform when calculating outlet stream conditions and properties. A value of 1 indicates an isothermal (constant temperature) flash and a value of 2 indicates an adiabatic (constant enthalpy) flash. For the adiabatic flash option only, a heating or cooling duty can be included in the outlet stream(s) calculation. The value should be stored in EQPAR(4). If you plan to use position 2 of the EQPAR list in your ADD block calculations, simply store the value in a temporary variable BEFORE calling the DESIGN II flash algorithm, then restore it afterwards. For example

```
SUBROUTINE XYZ(ARG1, ARG2, ARG3)
  ARG1=EQPAR(2)*EQPAR(6)/EQPAR(3)
  ARG2=ARG1**2
  ARG3=(ARG2+ARG4)*0.4/62.3
  SAVPAR=EQPAR(2)
  EQPAR(2)=1
  CALL FLASH1(NIN,NOUT,NCP,NEQP,NDSP,etc.)
  .
  .
  .
  EQPAR(2)=SAVPAR
```

---

### In a FORTRAN Library

---

If the same calculation needs to be performed in several equipment modules or you are creating an ADD block, you can define FORTRAN subroutine(s) which can be CALLED. These subroutine are grouped in a library which must be the last section of the input file. The commands used to define the library are:

FORTRAN

Define the special section where the FORTRAN statements will be placed; must be the last section of input file.

BLOCK j = number, name1, name2, ....

Identify the various sets of subroutines which are to be used with a specific ADD Block, where

j is a unique number for this Block,  
number is the count of subroutines used in this Block,  
name1,name2, are the names of subroutines used in this Block

STArt LIBrary

Indicates the beginning of standard FORTRAN statements; columns 1-5 are statement numbers, column 6 indicates continuation of previous line (up to 10 lines) and columns 7-72 are for FORTRAN statements. "C" in column 1 indicates a comment line.

STOp LIBrary

Indicates the end of FORTRAN statements.

The first subroutine name in the BLOCK j command should be the "driver" subroutine. It will control calculations and call the other subroutines within the BLOCK. The BLOCK command is only used with ADD block modules. The example *Inline FORTRAN: Railroad Tankcar Volume Calculation* shows usage of a FORTRAN library without an ADD Block.

---

## Add Inline FORTRAN Statements

---

Once you have reviewed all the parameters, subroutines, etc. available from Inline FORTRAN, set up your FORTRAN statements wherever they are appropriate - in equipment module(s), ADD blocks, or the FORTRAN LIBrary section. FORTRAN statements can appear in all three locations within one simulation.

Assign variable names, where needed, in your Inline FORTRAN statements. FORTRAN variable names may be up to 6 characters in length. Names beginning with I, J, K, L, M, and N are presumed to be integer variables (or arrays) unless they are specifically declared to be REAL. Remember to assign a length to all arrays.

For example, F- DIMENSION I(40), FCALC(40), RESULT(10)

---

## Add Optional FORTRAN Commands

---

Consider using optional FORTRAN commands. DEBUG LIMIT checks for proper dimensioning of vectors (arrays).

If your input file contains a FORTRAN LIBrary, you should consider storing the compiled and linked FORTRAN code in an external file. This file can be reused for subsequent runs without repeating all the code in the FORTRAN LIBrary. To save, use the following commands (the BLOCK command is for illustration only):

```
FORTRAN LIBrary  
BLOCK 1=4,MAIN1,AUX1,CALC1,PROP1  
NEW FOR FIL=SAVE,CODE,HERE  
START LIBrary
```

When you need to use the FORTRAN library again, simply refer to the external file where the code is stored. For example,

```
FORTRAN LIBrary  
BLOCK 1=...  
OLD FOR FIL=SAVE,CODE,HERE
```

If you need to add or change the FORTRAN LIBrary code which is stored in the external file, simply include the changes below the START LIBrary command and append a comma and the numeral 3 after the FORTRAN SAVE FILE name.

e.g. OLD FOR FIL=SAVE,CODE,HERE,3.

The names SAVE, CODE, HERE are examples only. You may use any three four-character names that you want to name your FORTRAN file.

Each name should begin with a letter; the remaining three characters of each name can be any alphanumeric character. Do not use commas, decimals, colons, semi-colons, or underline characters in these names.

---

## Inline Fortran: Review FORTRAN Coding

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Check your coding for situations which might result in an attempt to divide by zero or take the square root of a negative number. These are illegal operations which usually result in a halt to calculations. Make any conditional tests separate from GET or SET statements. Check that the variable names used in calculations match the spelling of the variable names in WRITE statements. Be sure that the formatting options for values match the variable type (REAL, INTEGER).

If there are problems with your Inline FORTRAN coding, the DESIGN II output file will contain a FORTRAN COMPILATION and LINKAGE section (just below ECHO PRINT OF INPUT DATA) which will provide you will a numbered listing of each subroutine (each set of equipment module FORTRAN commands is treated as a "subroutine"). The error messages will refer to the FORTRAN statement number(s) with which it is having difficulty processing. Incorrect syntax or mismatch in variable

## Chapter 18

names or types are the most common problems encountered. Be sure parentheses are balanced.

Beginning the FORTRAN commands in the wrong column can lead to incorrect interpretations. Be sure to leave 6 blank spaces between the F- and the beginning of a FORTRAN statement in the equipment module command sections. FORTRAN statement numbers may occur in columns 3-7. No FORTRAN statement should extend past column 74. Continue the statement on the next line, placing a continuation character in column 8.

Within the FORTRAN library section (between START LIBRARY and STOP LIBRARY commands, FORTRAN statements should be preceded by 6 blank spaces, continuation characters should be placed in column 6, and FORTRAN statement numbers may occur in columns 1-5. Coding should end by column 72 or be continued on the next line.

Also refer to *Table 1. Inline FORTRAN Restrictions* to ensure that you are not using an option which is not supported by Inline FORTRAN or FORTRAN 66.

### Inline FORTRAN Parameters, Module Functions, and Property Banks

#### Inline Fortran: General Parameters

DESIGN II allows user access to a wide range of parameters and properties from equipment modules, streams, and data banks for use in Inline FORTRAN. Values which will be retrieved or stored will be in DESIGN II internal dimensional units. Exceptions will be noted in the Tables.

<u>Category</u>	<u>Unit Label</u>
Temperature	degrees R
Pressure	psia
Enthalpy	Btu/hr
Length	feet
Time	hours
Quantity	lbmol (except where noted)
Density	lbmol/ft <sup>3</sup>
Work	horsepower

#### Parameters

The keyword commands to be used for retrieving or storing equipment module specifications and calculated properties in Inline FORTRAN are located in *Inline Fortran: Table 2. Flowsheet Parameters Available to GET and SET*. You are not allowed to SET the value of a calculated property. Some equipment module keyword commands allow more than one value (PRODUCTS from DISTILLATION columns, PRESSURE of STAGES for COMPRESSOR). These items will require an index to indicate the specific value you are trying to GET or SET.

Examples:

```
F-      SET (COMPRES (10), WOR AVA) = GET (EXP (3), CAL WOR) * 0.98
F-      TOTDUT = GET (DIS (5), CAL REB) + GET (DIS (5), HEA (1))
F-      SET (HEAEXC (17), DUT) = -TOTDUT
```

#### Inline Fortran: Stream Properties

The keyword commands to be used for retrieving or storing stream properties in Inline FORTRAN are located in *Inline Fortran: Table 2. Flowsheet Parameters Available to GET and SET*. Use caution in SETTING stream properties such as flowrate, temperature, or pressure for any stream which is not a feed stream to the flowsheet.

Examples:

```
F-      C1FRAC = GET (STR (10), FLOCOM (3)) / GET (STR (10), FLO)
F-      FLOLIQ = GET (STR (85), FLO) * (1.0 - GET (STR (85), VAP FRA))
F-      FLOMAS = FLOLIQ * GET (STR (85), MOL WEI LIQ)
F-      RHOLIQ = FLOMAS / GET (STR (85), VOL LIQ)
```

#### Inline Fortran: Distillation Functions

The distillation functions require the rigorous DISTILLATION column module, using SUPER or SUPER PLUS convergence options. These functions are only available DURING calculation of the DISTILLATION module. These functions are entered directly in the Inline FORTRAN commands (no GET/SET). See *Inline Fortran: Table 3. DISTILLATION Function* and Example 2 in *Inline Fortran: Reid Vapor Pressure Column Specification* for details of the Distillation functions.

Stage numbering is inverted during column calculations; the bottom stage is numbered 1. Stages for SUPER and SUPER PLUS are always trays + 2.

The normal coding for the DISTILLATION module must contain at least one product composition specifications (PURITY, RECOVERY or RATIO). This specification will be replaced by your EPS(1) specification which is defined using Inline FORTRAN. This

allows you to create your own DISTillation specifications. You may use GET/SET commands and other DESIGN II subroutines such as DENSTY or REIDVP to create these specifications. For columns requiring two heat and material balance specifications, you can define both an EPS(1) and EPS(2) specification. Your DISTillation commands should contain 2 product composition specifications in this case. Each EPS(i) specification should be defined such that its value is 0.0 when the specification is met. The error can be on a relative or absolute basis. For example, using the FLOWL(i,j) function,

Relative basis:

```
PURity BOTtom 2=0.015
F-      DURING
F-      CALL REICRU (FLOWL(1,1),RVP,IERR,ERR)
F-      EPS(1)=(RVP - 10.)/10.
```

Absolute basis:

```
PURity BOTtom 2=0.015
F-      DURING
F-      CALL REICRU (FLOWL(1,1),RVP,IERR,ERR)
F-      EPS(1)= RVP - 10.
```

## Inline Fortran: Pure Component Physical Property Data

Several pure component properties are available for use in Inline FORTRAN calculations. Each of these is stored in a data bank in the same order in which the components are listed in the COMponents command in the GENeral section. You must provide the bank name and the position(s) of the component(s) for which you want to retrieve data. Data is frequently retrieved from these banks by using a DO loop to walk across the component list. For example, if you wanted to calculate the mass fraction of the second component in Stream 5 (total components = 5), you would code the following:

```
F-      TOTMAS=0.0
F-      DO 25 I = 1,5
F-      TOTMAS= GET (STR(5), FLO COM(I)) *GET (BANK (AMW, POS (I))
F-      *+ TOTMAS
F- 25 CONTINUE
F-      C2MAS = GET (STR(5), FLO COM(2)) * GET (BANK (AMW, POS (2))
F-      C2FRA=C2MAS/TOTMAS
```

See *Inline Fortran: Table 4. Component Point Properties Subroutines Critical Point Values* and Example 9 in *Inline Fortran: Point Properties and Name Retrieval* for details of the pure component property banks.

## Inline Fortran: DESIGN II Utility Subroutines

There are several utility subroutines available in Inline FORTRAN. These routines handle pagination, copying and initializing stream properties at new conditions, and a convergence algorithm for solving iterative calculations. See *Inline Fortran: Table 5. Utilities Subroutine (use with Call)* and Example 8 in *Inline Fortran: Referencing Internally Calculated Streams* for details.

## Inline Fortran: Thermodynamic Library Subroutines 1

Twelve mixture property subroutines are available for use in Inline FORTRAN. You may use them to print out tables of properties at set conditions or combine them with FORTRAN statements to perform desired calculations. For the K-value, enthalpy, and density routines, the same thermodynamic equation option(s) which were selected in the GENeral section or the specific equipment module will be used to calculate those properties. For example, if the GENeral section contains the following keyword commands:

**PENK, PENH, STDD,**

then the Peng-Robinson equation of state would be used to calculate K-values and enthalpies, and the Yen-Woods equation would be used to calculate densities. Likewise, if thermodynamic choices have been made in the equipment module keywords, then those choices will be used for any thermodynamic subroutines which are called in that module. See *Inline Fortran: Table 6. Thermodynamic Library Subroutines (use with CALL)* and Example in *Inline Fortran: Railroad Tankcar Volume Calculation*

## Inline Fortran: Thermodynamic Interaction Parameter Banks

Several K-value correlations use binary interaction parameters to model non-ideal mixtures. These parameters are normally available from DESIGN II data banks (two tables for Peng-Robinson, one table for Lee-Kesler-Ploecker, one table for Benedict-Webb-Rubin-Starling) or are loaded from data regressions in ChemTran. You can use Inline FORTRAN to set the values of these parameters (and related properties) in the appropriate banks. There are specific bank names for the K-value options (e.g. WREN for RENon, WWIL for WILson) and a matrix position for the binary parameter (or property, such as R, Q and Q' parameters for UNIQUAC, molar volume ratio for WILson). See *Inline Fortran: Table 7. Thermodynamic Interaction Parameters* for details.

**NOTE:** Even though the RENon equation C12 and C21 parameters are equal, values for both must be entered when using Inline FORTRAN.

---

## Inline Fortran: DESIGN II Flash Subroutine

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This subroutine is used by ADD block modules to calculate outlet stream properties and phase distribution. If multiple inlet streams have been linked to the ADD block, they will be adiabatically mixed and flashed at the lowest feed pressure. Phase separation for the ADD block outlet streams will occur if the user has linked either 2 or 3 product streams to the ADD block. Either isothermal (constant temperature) or adiabatic (constant heat) flashes can be performed.

A complete description of the FLASH1 argument list is shown in *Inline Fortran: Table 8. DESIGN II Flash Subroutine (use with CALL)* Example 4, *Inline Fortran: Aircooled Exchanger ADD Block* illustrates the use of this subroutine.

## Inline FORTRAN Operators, Functions, and Keywords

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### Inline Fortran: Arithmetic Operators

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Operator	Name
=	Equals sign
+	Addition or Identity
-	Subtraction or Negation
*	Multiplication
/	Division
**	Exponentiation
(	Left Parenthesis
)	Right Parenthesis
OperatorPriority	
**	Highest
* and /	..
+ and -	Lowest

---

### Inline Fortran: Intrinsic Functions

---

Functions	Description
IABS	absolute value of a integer, I = IABS (I)
ABS	absolute value of a real, R = ABS (R)
SQRT	square root, R = SQRT (R)
AINT	truncate real, result is real, R = AINT (R)
INT	convert real to integer, I = INT (R)
IFIX	convert real to integer, I = IFIX (R)
FLOAT	convert integer to real, R = FLOAT (I)
MOD	remainder of calculation, integer, I = MOD (I1, I2)
AMOD	remainder of calculation, real, R = AMOD (R1, R2)
ISIGN	transfer of sign, integer, result is positive of first argument if second argument is positive, result is negation of first argument if second argument is negative, I = ISIGN (I1, I2)
SIGN	transfer of sign, real, result is positive of first argument if second argument is positive, result is negation of first argument if second argument is negative, R = SIGN (R1, R2)
IDIM	positive difference, integer, result is difference if first argument is greater than second argument, otherwise the result is zero, I = IDIM (I1, I2)
DIM	positive difference, real, result is difference if first argument is greater than second argument, otherwise the result is zero, R = DIM (R1, R2)
MAX0	greater of two arguments, integer, I = MAX0 (I1, I2)
MIN0	lesser of two arguments, integer, I = MIN0 (I1, I2)
AMAX	greater of two arguments, real, R = AMAX (R1, R2)
AMIN	lesser of two arguments, real, R = AMIN (R1, R2)
MAX1	greater of two real arguments, I = MAX1 (R1, R2)
MIN1	lesser of two real arguments, I = MIN1 (R1, R2)
AMAX0	greater of two integer arguments, R = AMAX0 (I1, I2)



AMIN0	lesser of two integer arguments, R = AMIN0 (I1, I2)
ALOG	natural logarithm, argument must be > zero, R = ALOG (R)
ALOG10	common logarithm, R = ALOG10 (R)
EXP	exponential, e**a, R = EXP (R)
SIN	sine, units are radians, R = SIN (R)
COS	cosine, units are radians, R = COS (R)
TANH	tangent, unit are radians, R = TANH (R)
ATAN	arctangent, units are radians, R = ATAN (R)
ATAN2	arctangent of argument 1 and argument 2 with respect to the sign of both arguments, units are radians, R = ATAN2 (R, R)

## Inline Fortran: Keywords

### Nonexecutable (specification, format specification, subprogram) Statements

DATA /...../	to initialize variables and array elements
REAL	data type statement
COMMON /...../	to define common variable names, array names, and array declarators
INTEGER	data type statement
LOGICAL	data type statement
DIMENSION	array declaration statement
SUBROUTINE	a routine which performs a calculation procedure and returns the results

### Executable (assigned, control, input/ouput) Statements

CALL	a SUBROUTINE is referenced with this statement.
RETURN	statement causes program control to be returned to the referencing program unit
DO	statement used to establish a controlled loop, specify the control variable, give the indexing parameters, and delineate range of loop
IF	conditional branching or statement execution based on the value of an arithmetic or logical expression
GOTO	transfer of control on an unconditional assigned, or computed basis
CONTINUE	statement serves as a point of reference. no operational function is performed
STOP	program execution is terminated
END	statement denotes the end of a FORTRAN program

### Input and Output Keywords

READ	statement used for formatted and unformatted input from the device
PRINT	used for formatted output to the system output device
DISPLAY	similar in function to print statement
FORMAT	statement used to establish a format specification
WRITE	statement used for formatted and unformatted output to the specified device

## Inline Fortran: Relational and Logical Operators

Relational Operators	Description
.EQ.	Equal to
.NE.	Not equal to
.GT.	Greater than
.GE.	Greater than or equal to
.LT.	Less than
.LE.	Less than or equal to

Logical Operators	Description
.NOT.	Logical negation

## Chapter 18

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.AND.	Logical conjunction
.OR.	Logical inclusive disjunction
.TRUE.	Boolean affirmation
.FALSE.	Boolean negation

---

### Inline Fortran: Input and Output Units

---

DESIGN II uses the following Fortran Input / Output Units for file manipulation:

- 1 - The DESIGN II input file
- 2 - The DESIGN II output file
- 4 - The DESIGN II keyword file, DESIDATA.FIL
- 5 - The console input (usually keyboard)
- 6 - The console output (usually monitor screen or window)
- 15 - Temporary scratch file
- 16 - Temporary scratch file
- 17 - Temporary scratch file
- 18 - Temporary scratch file
- 20 - Temporary scratch file
- 21 - Temporary scratch file
- 22 - Temporary scratch file
- 25 - Temporary scratch file
- 27 - Temporary scratch file
- 28 - Temporary file for holding DESIGN II Index of Flowsheet Calculations
- 29 - Temporary scratch file
- 30 - Temporary scratch file for smashing input
- 36 - Chemical file
- 37 - Stream file
- 38 - DesignMaster interface file
- 39 - Inline Fortran file
- 40 - Step Mode file
- 41 - Sequential Formatted Input file (LIQCONSOLE interface file)
- 42 - Sequential Formatted Input file (Inline Fortran library file)
- 43 - Direct Access Input file (Restart Read file)
- 44 - Direct Access Input file (Restart Write file)

### Inline Fortran Examples

There are several sample flowsheets in "Chapter 44: Inline Fortran Samples- C:\designii\samples\fortran" of the DESIGN II for Windows Tutorial and Samples Guide.

### Inline Fortran: Table 1. Inline FORTRAN Restrictions

Inline FORTRAN is an implementation of FORTRAN 66 internal to DESIGN II. However, it is not a full implementation and there are a few restrictions. Within these restriction, it possesses all of the flexibility of the FORTRAN IV language. The restrictions are:

1. EQUIVALENCE statements are not available.
2. LOGICAL statements and logical variables cannot be used.
3. The FORTRAN function routine cannot be used.
4. The FORTRAN functions MAX0, MAX1, MIN0, and MIN1 can only be used with two arguments.
5. FORTRAN 77 extensions (WHILE, ELSE,...) are not available.
6. The maximum number of characters on each line for FORTRAN statements is 74; including the F-, comment (C), statement number, and continuation columns.
7. Up to 10 continuation lines are allowed, using the standard FORTRAN convention of a character in the sixth column to indicate continuation.
8. Only one variable, scalar or vector per DATA statement is allowed.
9. COMMON variables cannot be initialized by a DATA statement.
10. Subscripts cannot have subscripts.

Several DESIGN II library and utility subroutines are available for use with Inline FORTRAN. The DESIGN II subroutines do not require the INCLUDE subroutine name command to be CALLED. A few special DISTillation functions (for use "DURING" calculations) and several component point properties are also available.

**Inline Fortran: Table 2. Variables Available to GET and SET**

A complete list of equipment parameters and stream properties which can be accessed by GET and SET (and also used in Flowsheet Optimization) is shown below. The parameters shown are also available in OPTIMization and in the CASestudy commands TABLE, PLOTX, and PLOTY. The dimensional units shown are the DESIGN II internal units in which the item will be stored. Those items highlighted in **gray** are **NOT** available to the Inline FORTRAN SET command and the CASestudy STEp and CHAnge commands.

**STReam properties**

CP IMM	Heat capacity at constant pressure for immiscible portion of stream	BTU/LBMOL/R
CP LIQ	Heat capacity at constant pressure for liquid portion of stream	BTU/LBMOL/R
CP VAP	Heat capacity at constant pressure for vapor portion of stream	BTU/LBMOL/R
CV IMM	Heat capacity at constant volume for immiscible portion of stream	BTU/LBMOL/R
CV LIQ	Heat capacity at constant volume for liquid portion of stream	BTU/LBMOL/R
CV VAP	Heat capacity at constant volume for vapor portion of stream	BTU/LBMOL/R
ENTH	Total stream enthalpy	BTU/HR
ENTH IMM	Enthalpy of immiscible portion of stream	BTU/HR
ENTH LIQ	Enthalpy of liquid portion of stream	BTU/HR
ENTH VAP	Enthalpy of vapor portion of stream	BTU/HR
ENTR	Total stream entropy	BTU/HR
ENTR IMM	Entropy of immiscible portion of stream	BTU/HR
ENTR LIQ	Entropy of liquid portion of stream	BTU/HR
ENTR VAP	Entropy of vapor portion of stream	BTU/HR
<b>FLO</b>	<b>Stream flowrate</b>	<b>LBMOL/HR</b>
<b>FLO COM (i)</b>	<b>Flowrate for "ith" component</b>	<b>LBMOL/HR</b>
<b>FLO IMM COM</b>	<b>Immiscible component flowrate</b>	<b>LBMOL/HR</b>
<b>MAS FLO</b>	<b>Stream Mass flowrate</b>	<b>LB/HR</b>
MOL WEI	Stream average molecular weight	----
MOL WEI IMM	Molecular weight of immiscible portion of stream	----
MOL WEI LIQ	Molecular weight of liquid portion of stream	----
MOL WEI VAP	Molecular weight of vapor portions of stream	----
NUM PHA	Number of phases	----
<b>PRE</b>	<b>Stream pressure</b>	<b>PSIA</b>
REI VAP PRE	Reid vapor pressure	PSI
SUR TEN	Surface tension of liquid portion of stream	DYNES/CM
SUR TEN IMM	Surface tension of immiscible portion of stream	DYNES/CM
<b>TEM</b>	<b>Stream temperature</b>	<b>R</b>
THE CON IMM	Thermal conductivity of immiscible portion of stream	BTU/FT/HR/R
THE CON LIQ	Thermal conductivity of liquid portion of stream	BTU/FT/HR/R
THE CON VAP	Thermal conductivity of vapor portion of stream	BTU/FT/HR/R
UOPK	UOP K factor	
VAP FRA	Molar vapor fraction	----
VIS IMM	Viscosity of immiscible portion of stream	CENTIPOISE
VIS LIQ	Viscosity of liquid portion of stream	CENTIPOISE
VIS VAP	Viscosity of vapor portion of stream	CENTIPOISE
VOL	Total stream volume at system temperature and pressure	FT3/HR
VOL IMM	Volume of immiscible portion of stream at system temperature and pressure	FT3/HR
VOL LIQ	Volume of liquid portion of stream at system temperature and pressure	FT3/HR
VOL VAP	Volume of vapor portion of stream at system temperature and pressure	FT3/HR
Z IMM	Compressibility factor for immiscible portion of stream	----
Z LIQ	Compressibility factor for liquid portion of stream	----
Z VAP	Compressibility factor for vapor portion of stream	----

**CRUde Stream Properties**

ASTM IBP	D 86 initial boiling point	F
ASTM 5PT	D 86 5% point	F
ASTM 10PT	D 86 10% point	F
ASTM 30PT	D 86 30% point	F
ASTM 50PT	D 86 50% point	F
ASTM 70PT	D 86 70% point	F
ASTM 90PT	D 86 90% point	F
ASTM 95PT	D 86 95% point	F
ASTM EP	D 86 end point	F
CUM VOL (i)	Cumulative volume	VOLUME %
FLA	Flash point	R
FLO	Molar flow rate	LBMOL/HR
POUR	Pour point	R
PRO SET (i)	Total stream property calculated on a molar basis	----
PRO SET WEI (i)	Total stream property calculated on a weight basis	----
PRO SET VOL (i)	Total stream property calculated on a volume basis	----
SP GR	Specific gravity	SPG
TBP IBP	TBP initial boiling point	F
TBP 5PT	TBP 5% point	F
TBP 10PT	TBP 10% point	F
TBP 30PT	TBP 30% point	F

# Chapter 18

TBP 50PT	TBP 50% point	F
TBP 70PT	TBP 70% point	F
TBP 90PT	TBP 90% point	F
TBP 95PT	TBP 95% point	F
TBP EP	TBP end point	F
VABP	Volume average boiling point	R
VIS SET (i)	The "ith" set of viscosity data at set temp	CST
VOL	Volumetric flow rate at stream temperature and pressure	FT3/HR

\*LBMOL/HR, LB/HR, OR GAL/HR depending upon input being molar, mass or volumetric units

<b>Module/Keyword</b>	<b>Parameter Description</b>	<b>Units</b>
-----------------------	------------------------------	--------------

**ADD block**

**EQPar (i)** "ith" parameter for ADD block equipment list

\*

- as defined by user

**AIR Cooler**

**DUT** Duty

BTU/HR

**CAL DUT** Calculated Duty

BTU/HR

**Amine Column**

**NONE\*** No variables of the Amine Column are available

n/a

**NOTE:** \* Similar to other unit modules Inline Fortran can be used for PRE/POST calculations.

**COMPONENT SPLITTER**

**REC TOP(i)** Flowrate or fraction of "ith" component in 1st outlet

\*

**TEM BOT** Temperature of second outlet

R

**TEM COO** Temperature of cooling fluid

R

**TEM HEA** Temperature of heating fluid

R

**TEM TOP** Temperature of first outlet

R

\*Default is molar fraction, otherwise flow units as specified in input.

**COMPRESSOR**

**CAL ELE** Calculated electricity usage

KW

**CAL FUE** Calculated fuel gas usage

SCF/HR

**CAL POL** Calculated polytropic coefficient

----

**CAL STE** Calculated steam usage

LB/HR

**CAL WAT** Calculated cooling water (multistage)

GAL/HR

**CAL WOR** Calculated work required

HP

**DUT INT (i)** "ith" stage intercooler duty

BTU/HR

**EFF** Efficiency

----

**POL COE** Polytropic coefficient

----

**POL HEA** Polytropic head

FT

**POL STA (i)** "ith" stage polytropic coefficient

----

**POLytropic FLAg** Polytropic head

0 = User input value,  
1 = Calculate in program

**PRE OUT** Final discharge pressure

PSIA

**PRE STA (i)** Discharge pressure for stage (i)

PSIA

**STA** Number of stages (10 maximum)

----

**STE IN** Driver inlet steam enthalpy

BTU/LBMOL

**STE OUT** Driver outlet steam enthalpy

BTU/LBMOL

**TEM BUB** Temperature for spec PRE OUT at BUB PT

R

**TEM DEL (i)** "ith" stage delivery temperature

R

**TEM DEW** Temperature for spec PRE OUT at DEW PT

F

**TEM INT** Temperature interstage cooler

R

**TEM SUC (i)** "ith" stage suction temperature

R

**VAP WT (i)** "ith" stage mass flow rate

LB/HR

**VOL SUC (i)** "ith" stage suction volumetric Flow

FT3/HR

**WOR AVA** Available work

HP

**WOR STA (i)** "ith" stage work

BTU/HR

Only one of these three will be calculated per compressor as determined by the input keyword.

**DEPRESSURING**

**BAC** Backpressure

PSIA\*

**COE** Coefficient of discharge

----

**CRO** Cross section of valve

FT2

**DIA** Diameter of vessel

FT

**ENV** Environment factor

----

**HEA** Heat addition

BTU/HR

**RED** Final pressure after blowdown

PSIA

**SET** Set pressure for valve to open

PSIA

**LEN** Length of vessel

FT

**LIQ HEI** Liquid height

FT

**TIM STE** Time step

HR

**DISTILLATION**

**CAL DUT CON** Calculated condenser duty

BTU/HR

<b>CAL DUT REB</b>	Calculated reboiler duty	BTU/HR
<b>CAL DUT INT(i)</b>	Calculated "ith" intercooler duty	BTU/HR
<b>CAL MAX DIA</b>	Maximum diameter from Smith-Dresser Ohlswager	FT2
<b>CAL NOR</b>	Norm (error analysis)	----
<b>CAL PRO (i)</b>	Calculated "ith" product	*
<b>CAL REF</b>	Calculated reflux ratio	----
<b>CAL TEM TOP</b>	Calculated temperature for top product	R
<b>CAL TEM BOT</b>	Calculated temperature for bottom product	R
<b>CAL TEM PRO (i)</b>	Calculated temperature profile for each "ith" tray	R
<b>COM CON (i)</b>	Compositional convergence	----
<b>DEC COM</b>	Decant component identification number	----
<b>DEC RAT</b>	<b>Estimate for decant rate</b>	LBMOL/HR
<b>DEC REF</b>	Molar fraction solubility in reflux	----
<b>DEL</b>	Pressure drop through column	PSI
<b>DTS</b>	Change in delta temperature for column profiles (convergence control)	----
<b>DUT CON</b>	Specified condenser duty	BTU/HR
<b>DUT INT(i)</b>	Duty of the "ith" Intercooler or side-reboiler	BTU/HR
<b>DVS</b>	Change in delta V for profile; average factor (SUPER)	----
<b>EXT COM</b>	Identification number for extractive component	----
<b>HEA (i)</b>	Heat added/removed from "ith" heater/cooler	BTU/HR
<b>HEA KEY</b>	Heavy key component identification number	----
<b>IMM</b>	Immiscible component identification number	----
<b>LIG KEY</b>	Light key component identification number	----
<b>LIQ PRO (i)</b>	'ith' stage liquid	LBMOL/HR
<b>LOC FEE (i)</b>	Feed tray location for "ith" feed	----
<b>LOC HEA (i)</b>	Heater/cooler location for "ith" heater	----
<b>LOC INT (i)</b>	Location for "ith" intercooler	----
<b>LOC SID (i)</b>	Location of "ith" side draw	----
<b>MAX DIM</b>	Maximum dimension for matrix	----
<b>MAX MAT</b>	Maximum number of matrix inversions	----
<b>PRE CON</b>	Condenser pressure	PSIA
<b>PRE TOP</b>	Top tray pressure	PSIA
<b>PRI SWI</b>	Column output print control	----
<b>PRO (i)</b>	Rate for "ith" product	LBMOL/HR
<b>REB</b>	Specified reboiler duty	BTU/HR
<b>REF</b>	Reflux ratio	----
<b>REF GUE</b>	Guess for reflux ratio	----
<b>SPE (i)</b>	"ith" SUPER specification	----
<b>TEM BOT</b>	Guess for bottom product temperature	R
<b>TEM CHI</b>	Presaturator chiller temperature	R
<b>TEM CON SUB</b>	Degrees of subcooling for total condenser	R
<b>TEM CON</b>	Condenser temperature	R
<b>TEM INT (i)</b>	Temperature for "ith" intercooler	R
<b>TEM PRO (i)</b>	"ith" value from temperature profile	R
<b>TEM REB</b>	Specified reboiler temperature	R
<b>TEM TOP</b>	Guess for bottom product temperature	R
<b>THE</b>	Mole fraction vaporized from thermosiphon reboiler	----
<b>TOL</b>	Tolerance for column convergence	----
<b>TRA</b>	Number of trays	----
<b>TST</b>	Max temperature step, max % changes in vapor	----
<b>VAPPRO (i)</b>	"ith" value from vapor profile	LBMOL/HR

\*Default is lbmol/hr; if FRA specified, value is fraction of total feed.

\*\*RATio, RECover, PURity, and TOTal PROduct specification only.

### DIVider

**FLO RAT i** Flowrate of "ith" outlet \*

\*Default is molar fraction; otherwise flow units as specified by user in input.

### Double Pipe HEAt EXChanger

**NONE\*** No variables of the Double Pipe Heat Exchanger are available n/a

**NOTE:** \* Similar to other unit modules Inline Fortran can be used for PRE/POST calculations.

### EQUilibrium REActor

**EXT (i)** Extent completion of reaction number i ----

**INE (i)** ID number of "ith" inert component ----

**TEM REA (i)** Approach to equilibrium temperature for reaction number (i) R

### EXPander

**CAL WOR** Calculated work produced HP

**EFF** Adiabatic efficiency ----

**PRE OUT** Final discharge pressure PSIA

### EXPander COMpressor

**NONE\*** No variables of the Expander Compressor/Pump are available n/a

### FIRed heater

# Chapter 18

CAL FUE	Calculated fuel usage	SCF/HR
CAL HEA ABS	Calculated heat absorbed	BTU/HR
DEL	Process stream pressure drop	PSI
EFF	Fuel efficiency	----
HEA VAL FUE	Heating value of fuel	BTU/LBMOL
RAT HEA	Rating of fired heater	BTU/HR
TEM OUT	Temperature of stream out	R
<b>FLAsh</b>		
CAL DUT	Calculated duty	BTU/HR
DEL	Pressure drop	PSI
HEA	Heat addition	BTU/HR
LIQ FRA	Specified liquid fraction	*
OIL ENT WAT	Fraction (W, M, V) oil in water	**
PRE OUT	Pressure	PSIA
TEM EXC	Temperature exchange	R
TEM OUT	Temperature	R
WAT ENT OIL	Fraction (W, M, V) water in oil	**
* mole fraction stored as (+), mass fraction stored as (-)		
** value <<10 implies mole fraction 10<<value<<20 implies mass fraction; true value = value -10. Value >>20 implies volume fraction; true value = value -20.		
<b>FMTR (Flow Meter)</b>		
FLO RAT	Flow Rate	LBMOL/HR
INS DIA	Inside Diameter	FT
NOM DIA	Nominal Diameter	FT
CAL FLO	Calculated Flowrate	LBMOL/HR
CAL DIA	Calculated diameter	FT
CAL DEL	Calculated delta pressure	PSIA
PRE LOS	Pressure Loss	PSIA
DIA	Diameter	FT
DEL	Delta pressure	PSIA
TYP	Type: SQUare-edged=1, QUAdrant=2, CONical=3	
TAP	Tap Type: FLAnge=1, CORner=2, RADius=3, PIPe = 4	
MET	Method: ISO=1, AGA=2, API=3	
RAT	Ratio	
Note:	Format: SET(FMTR(10),TYP) = 2 SET(FMTR(10),TAP)=4	
<b>HEAt EXChanger</b>		
ARE	Area	FT2
BAF CLE	Baffle clearance	FT
BAF CUT	Baffle cut	----
BAF SPA	Baffle spacing	FT
CUR INC	Curve increments	----
CAL ARE	Calculated area	FT2
CAL DUT	Calculated duty	BTU/HR
CAL WAT	Calculated cooling water for single stream exchanger	GAL/HR
DEL (i)	Pressure drop shell, tube	PSI
DEL TEM	1st outlet temperature - 1st inlet temperature	R
DUT	Duty	BTU/HR
EST ARE	Estimated Area	FT2
INL	Inlet flag	0 = Same, 1 = Opposite
LOG MEA TEM	Log mean temperature difference	R
NUM FEE 1	Number Shell Side Feeds	----
NUM FEE 2	Number Tube Side Feeds	----
MAX ITE	Maximum iteration for rating calculation	----
MIN TEM	Minimum temperature approach	R
NUM INC	Number of Increments	----
NUM TUB	Number of tubes	----
NUM SEA	Number of sealing strips	----
POS(112)-- THF	Tube Side Factor	----
POS(113)-- UFA	Overall Heat Transfer Factor	----
POS(114)-- SHF	Shell Side Factor	----
PRO 1	Shell Side Phase Separation	----
PRO 2	Tube Side Phase Separation	----
PRE REF	Pressure of refrigerant stream	PSIA
REF ID	Refrigerant identification number	----
SHE	Number of shells	----
SHE DIA	Shell diameter	FT
SHE FOU FAC	Shell fouling factor	1/(BTU/HR/FT2/R)
SHE PAS	Number of shell passes	----
TEM APP	2nd inlet temperature - 1st outlet temperature	R
TEM EXC	Temperature exchange	R
TEM OUT	Temperature out for 1st inlet stream	R
TEM REF	Temperature of refrigerant stream	R
TEM WAT IN	Temperature cooling water in	R
TEM WAT OUT	Temperature cooling water out	R

<b>TOL</b>	Tolerance for rating	----
<b>TUB BUN</b>	Tube bundle diameter	FT
<b>TUB BWG</b>	Tube BWG	----
<b>TUB FEE</b>	Tube feed	----
<b>TUB FOU</b>	Tube side fouling factor	1/(BTU/HR/FT <sup>2</sup> /R)
<b>TUB INS</b>	Tube inside diameter	FT
<b>TUB LAY</b>	Tube layout flag	1 = Triangular, 2 = Square, 3 = Rotated triangle, 4 = Rotated square
<b>TUB LEN</b>	Tube length	FT
<b>TUB OUT</b>	Tube outside diameter	FT
<b>TUB PAS</b>	Number of tube passes	----
<b>TUB PIT</b>	Tube pitch	FT
<b>TUB WAL</b>	Tube wall thickness	FT
<b>TUB FLO</b>	Flow direction flag	0 = Up, 1 = Down
<b>U</b>	Heat transfer coefficient	BTU/HR/FT <sup>2</sup> /R
<b>VER</b>	Vertical flag	0 = Horizontal, 1 = Vertical

### HYdroTReater

<b>ARO CON</b>	Aromatic mole fraction converted	----
<b>ARE REA</b>	Fraction aromatics converted to saturated hydrocarbons	----
<b>BED</b>	Estimated number of beds	----
<b>CON DRO</b>	Temperature drop between beds	R
<b>CON RIS</b>	Temperature rise between beds	R
<b>MAX</b>	Maximum number of beds	----
<b>NIT CON</b>	Nitrogen weight fraction	----
<b>NIT REA</b>	Fraction nitrogen converted to ammonia	----
<b>OLE CON</b>	Olefin mole fraction	----
<b>OLE REA</b>	Fraction olefins converted to saturated hydrocarbons	----
<b>OPT DRO</b>	Temperature drop option (0, 1)	----
<b>OPT QUE</b>	Quench option (0, 1)	----
<b>OPT RIS</b>	Temperature control option (0, 1, 2)	----
<b>PRE DRO</b>	Pressure drop per bed (0, 1, 2)	----
<b>PRE QUE</b>	Pressure for quench stream	PSIA
<b>PRI</b>	Print option (0, 1, 2)	----
<b>SUL CON</b>	Sulfur weight fraction	----
<b>SUL REA</b>	Fraction sulfur converted to hydrogen sulfide	----
<b>TEM DRO (i)</b>	Temperature drop for OPT DRO = 1	R
<b>TEM QUE</b>	Temperature of quench stream	R
<b>TEM RIS (i)</b>	Temperature rise per bed	R

### LINE pressure drop

<b>CAL DEL FRI</b>	Calculated delta pressure due to friction	PSI
<b>CAL DEL ELE</b>	Calculated delta pressure due to elevation	PSI
<b>CAL U n</b>	Calculated U factor	BTU/HR/FT <sup>2</sup> /F
<b>CAL UPS PRE</b>	Calculated Upstream pressure	PSIA
<b>CON m, SEG n</b>	Insulation Layer Conductivity per Segment	BTU/HR/FT/F
<b>DRA</b>	Drag	----
<b>EFF</b>	Efficiency	----
<b>ELE (i)</b>	"ith" node pure elevation	FT
<b>EQV (i)</b>	"ith" node equivalent length	FT
<b>FLO DIR</b>	Flow direction	flag
<b>INS DIA (i)</b>	"ith" node inside diameter	FT
<b>INS m, SEG n</b>	Insulation Layer Thickness per Segment.	FT
<b>LEN (i)</b>	"ith" node length	FT
<b>LIQ HOL (i)</b>	"ith" node liquid holdup	----
<b>NOM DIA (i)</b>	"ith" node nominal diameter	FT
<b>PIP DEP n</b>	Pipe Depth	FT
<b>PIP THI n</b>	Pipe Thickness	FT
<b>PRE OUT</b>	Outlet Pressure	PSIA
<b>TEM SUR (i)</b>	"ith" node temperature of surroundings	R
<b>ROU</b>	Roughness	FT
<b>SUR WAT CON n</b>	Surrounding Conductivity of Water	BTU/HR/FT/F
<b>SUR AIR CON n</b>	Surrounding Conductivity of Air	BTU/HR/FT/F
<b>SUR SOI CON n</b>	Surrounding Conductivity of Soil	BTU/HR/FT/F
<b>U (i)</b>	"ith" node heat transfer coefficient	BTU/HR/FT <sup>2</sup> /F
<b>VEL SUR n</b>	Velocity of Surrounding	FT/HR

'm' refers to layer number, 'n' refers to the segment number. See examples.

Example of format: variable = GET(LINE(no.), INSulation(mth layer),SEGment(nth segment))

### LNG exchanger

<b>ARE (i)</b>	Area per shell	FT <sup>2</sup>
<b>CAL ARE (i)</b>	Calculated area for tube i	FT <sup>2</sup>
<b>CAL DUT (i)</b>	Calculated tubeside duty	BTU/HR
<b>CAL DUT SHE (i)</b>	Calculated duty shell (i)	BTU/HR
<b>CAL DUT TUB (i)</b>	Calculated duty tube (i)	BTU/HR
<b>CAL LMT (i)</b>	Calculated LMTD (i)	R
<b>CAL MIX TEM</b>	Temperature shell feed after tubeside recycle	R

# Chapter 18

CAL TOT ARE	Calculated total area	FT2
CAL TOT DUT	Calculated total duty	BTU/HR
DEL SHE (i)	Pressure drop shell stream (i)	PSI
DEL TUB (i)	Pressure drop tube stream (i)	PSI
DUT (i)	Duty tubeside stream (i)	BTU/HR
REC STR	Number of tubeside streams recycled to shellside feed	----
SHE	Number of shells	----
SHE PAS	Number of passes per shell	----
SHE STR	Number of shellside streams	----
TEM APP (i)	Shell inlet temperature - tubeside outlet stream (i) temperature	R
TEM OUT (i)	Outlet temperature of tubeside stream (i)	R
TEM OUT SHE	Temperature out for shell stream(s)	R
TOT DUT	Shellside total duty	BTU/HR
TUB PAS	Number tube passes/shell	----
U (i)	Heat transfer coefficient for tubeside stream (i)	BTU/HR/FT2/F

**NOTE:** The stream position number is (i). Recycle tubeside stream(s) are coded as the first stream(s). Next, the remaining tubeside stream(s) are coded. Finally, the shellside stream(s) are coded. Only one shellside stream is allowed if any tubeside stream is recycled.

## MASs BALance

**NONE\*** No variables of the Mass Balance are available n/a

## PACKed COLumn

**NONE\*** No variables of the Packed Column are available n/a

## Plate-Fin EXchanger

**NONE\*** No variables of the Plate-Fin Exchanger are available n/a

**NOTE:** \* Similar to other unit modules Inline Fortran can be used for PRE/POST calculations.

## POLytropic compressor

CAL DIS TEM	Calculated discharge temperature	R
CAL DIS PRE	Calculated discharge pressure	PSIA
CAL POL EFF	Calculated polytropic efficiency	----
CAL POL HEA	Calculated polytropic head	HP
CAL SUC VOL	Calculated suction volume	FT3/MIN
PRE OUT	Outlet pressure	PSIA
SPE	Radial speed	RPM
THE FAC	Thermodynamic factor	----
TOL	Convergence tolerance	----

## PUMp

CAL ELE	Calculated electricity usage	KW
CAL FUE	Calculated fuel gas usage	SCF/HR
CAL STE	Calculated steam usage	LB/HR
CAL WOR	Calculated work required	HP
EFF	Efficiency	----
PRE OUT	Final discharge pressure	PSIA
STE IN	Driver inlet steam enthalpy	BTU/LBMOL
STE OUT	Driver outlet steam enthalpy	BTU/LBMOL
TEM BUB	Temperature for specification PRE OUT at BUB PT	R
TEM DEW	Temperature for specification PRE OUT at DEW PT	R
WOR AVA	Work available	HP

Only one of these three can be accessed per pump as determined by the module keywords: ELE DRI, FUEL, or STE IN/STE OUT.

## REFine

<b>General Column Parameters</b>		
LOC FEE (i)	Location of feeds	----
PRE CON	Pressure of condenser	PSIA
PRE TOP (i)	Pressure top (i)	PSIA
PRO (i)	Product rate	*
PRO GUE (i)	Product guess (i)	LBMOL/HR
PRO OVE	Product overhead rate	LBMOL/HR
PRO SPE (i)	Product Specification	----
REF RATI	Reflux ratio	MOLE FRACTION
REF RATE	Reflux Rate	LBMOL/HR
STA (i)	Stages	----
TEM BOT (i)	Temperature bottom	R
TEM CON	Temperature of condenser	R
TEM CON SUB	Temperature of condenser subcooling	R
TEM CON GUE	Temperature of condenser guess	R
TEM TOP (i)	Temperature top	R
WAT	Decanted water	LBMOL/HR
WAT DUT	Duty of condensed water	BTU/HR
<b>Fix Parameters</b>		
FIX GUE (i)	"ith" fix guess	LBMOL/HR
FIX LIQ (i)	"ith" fix liquid rate	LBMOL/HR



<b>FIX LIQ NET</b> (i)	"ith" fix liquid net rate	LBMOL/HR
<b>FIX TEM</b> (i)	"ith" fix temperature	R
<b>FIX VAP</b> (i)	"ith" fix vapor rate	LBMOL/HR
<b>Heater and Stripping Steam Parameters</b>		
<b>HEA</b> (i)	Heat added or removed	R
<b>LOC HEA</b> (i)	Tray location of heaters	----
<b>LOC STE</b> (i)	Tray location of steam	----
<b>PRE STE</b> (i)	Pressure of steam	PSIA
<b>STE</b> (i)	Steam rates	LBMOL/HR
<b>TEM STE</b> (i)	Temperature of steam	R
<b>Profile Parameters</b>		
<b>DEN LIQ</b> (i)	"ith" tray density liquid	LBMOL/FT3
<b>DEN VAP</b> (i)	"ith" tray density vapor	LBMOL/FT3
<b>ENT LIQ</b> (i)	"ith" tray enthalpy liquid	BTU/HR
<b>ENT VAP</b> (i)	"ith" tray enthalpy vapor	BTU/HR
<b>LIQ PRO</b> (i)	"ith" tray liquid	LBMOL/HR
<b>MOL WEI LIQ</b> (i)	"ith" tray molecular weight liquid	LB/LBMOL
<b>MOL WEI VAP</b> (i)	"ith" tray molecular weight vapor	LB/LBMOL
<b>NET LIQ</b> (i)	"ith" tray net liquid	LBMOL/HR
<b>PRE PRO</b> (i)	"ith" tray pressure	PSIA
<b>SP GR VAP</b> (i)	"ith" tray specific gravity vapor	SPG
<b>SP GR LIQ</b> (i)	"ith" tray specific gravity liquid	SPG
<b>TEM PRO</b> (i)	"ith" tray temperature	R
<b>VAP PRO</b> (i)	"ith" tray vapor	LBMOL/HR
<b>See: Inline Fortran: Table 9. REFIne Module Subroutines</b>		
<b>Pumparound Parameters</b>		
<b>CHA PUM</b> (i)	Change of pumparound temperature	R
<b>HEA PUM</b> (i)	Specified heat removed by pumparound (i)	BTU/HR
<b>CAL HEA PUM</b> (i)	Calculated heat removed by pumparound (i)	BTU/HR
<b>LOC PUM</b> (i)	Tray location of pumparounds	----
<b>LOC PUM WAT</b> (I)	Tray location of pumparounds for water	----
<b>CAL PRO PUM</b> (i)	Calculated flowrate by pumparound (i)	lbmol/hr
<b>PRO PUM</b> (i)	Specified product of pumparound	*
<b>TEM PUM</b> (i)	Temperature of pumparound	R
<b>Reboiler Parameters</b>		
<b>CAL REB</b> (i)	Calculated reboiler duty	BTU/HR
<b>REB</b> (i)	Reboiler duty	BTU/HR
<b>REB DEL</b> (i)	Reboiler return delta pressure	PSI
<b>REB EX VAP</b> (i)	Reboiler exit vaporization	WEIGHT%
<b>REB FLO</b> (i)	Reboiler flowrate	LBMOL/HR
<b>REB TEM</b> (i)	Reboiler temperature	R
<b>REB TYP</b> (i)	Reboiler type	----
<b>REB VAP GUE</b> (i)	Reboiler vapor guess	LBMOL/HR
<b>Side Stripper Parameters</b>		
<b>CHA RET</b> (i)	Change in return temperature	R
<b>DRA</b> (i)	Draw rates to stripper	LBMOL/HR
<b>HEA RET</b> (i)	Heat from liquid return	BTU/HR
<b>LOC DRA</b> (i)	Tray location of draws	----
<b>LOC LIQ</b> (i)	Tray location of liquid returns	----
<b>LOC VAP</b> (i)	Tray location of vapor returns	----
<b>PRO STR</b> (i)	Product from stripper	*
<b>PRO STR GUE</b> (i)	Product from stripper guess	LBMOL/HR
<b>RET</b> (i)	Return flow from stripper	LBMOL/HR
<b>TEM RET</b> (i)	Temperature of liquid return	R
<b>Tray Sizing Parameters</b>		
<b>GLI DIA</b> (i)	"ith" Glitsch diameter specification	FT
<b>GLI PER</b> (i)	"ith" Glitsch percent flood specification	%
<b>GLI PAS</b> (i)	"ith" Glitsch passes specification	----
<b>GLI SPA</b> (i)	"ith" Glitsch spacing specification	FT
<b>GLI SWA</b> (i)	"ith" Glitsch swage trays specification	----
<b>GLI SYS</b> (i)	"ith" Glitsch system factor specification	FRACTION
<b>Other Parameters</b>		
<b>CON FLAG</b>	Convergency flag	----
<b>MAX MAT</b>	Maximum matrices	----
<b>REP</b> (i)	Reports	----
<b>SWI</b>	Switch	----
<b>TOL</b>	Tolerance	----
<b>SHORtcut fractionator</b>		
<b>CAL DUT CON</b>	Calculated condenser duty	BTU/HR
<b>CAL DUT REB</b>	Calculated reboiler duty	BTU/HR
<b>CAL FEE TRA</b>	Calculated feed tray	----
<b>CAL MIN REF</b>	Calculated minimum reflux ratio (RR)	----
<b>CAL MIN STA</b>	Calculated minimum number of stages	----
<b>CAL REF</b>	(PER MIN) (CAL MIN REF)	----
<b>CAL STA</b>	Number stages at specified RR	----

## Chapter 18

DEL	Column pressure drop	----
PER MIN	Percent of minimum reflux ratio	----
PRE TOP	Column pressure at top	PSIA
REC BOT	Heavy key bottom product/heavy key feed	----
REC TOP	Light key top product/light key feed	----
TEM COO	Temperature of cooling fluid	R
TEM HEA	Temperature of heating fluid	R
TOT	Flag to denote condenser type	0 = Partial, 1 = Total

### STReam MANipulator

CAL MOL	Calculated value per LBMOL of input stream. For HEA VAL option, the calculated value is the heating value in BTU; when STR MAN is used to modify stream component flowrates, the calculated value corresponds to the total flowrate of the modified stream (i.e., second outlet stream) in LBMOL/HR.	VALUE/LBMOL
CAL SCF	Calculated value per SCF of input stream. The description of the calculated value is the same as for CAL MOL.	VALUE/SCF
FAC (i)	Factor by which "ith" component is to be ADDED SUBtracted, MULTiplied or DIVided.	----

### VALve

DEL	Pressure drop across valve	PSI
PRE OUT	Outlet pressure	PSIA
TEM BUB	Temperature for specified PRE OUT at BUB PT	R
TEM DEW	Temperature for specified PRE OUT at DEW PT	R

## Inline Fortran: Table 3. DIStillation Function

The distillation functions require the rigorous DIStillation column module, using the SUPer convergence option. These are **only** available DURING calculation of DIStillation module. The stage locations are inverted; the bottom stage is numbered 1. These functions are entered directly in Inline FORTRAN commands (no GET/SET).

Type/Name	Description
FLOWL (i,j)	Liquid flowrate of "ith" component, leaving stage "j" in lbmol/hr.
FLOWV (i,j)	Vapor flowrate of "ith" component leaving stage "j" in lbmol/hr.
TEM (j)	Temperature of "j" stage.
EPS (1)	Overrides first purity, ratio or recovery spec in input (user-defined units).
EPS(2)	Overrides second purity, ratio or recovery spec in input (user-defined units).

- NOTE:**
1. Stages for SUPer are always theoretical trays + 2. You can use these functions along with GET/SET commands and subroutines such as CALL DENSTY(...) to create any distillation specification desired. Use Inline FORTRAN to define EPS(1) and EPS(2) to zero when the desired specs are met. See Example 2.
  2. You must specify an EPS(1) specification to use these functions.
  3. If application has 2 PURity, RATio, or RECoverly specifications, both must be defined using EPS(1) for the first and EPS(2) for the second.

## Inline Fortran: Table 4. Component Properties (Tc,Pc,..) Subroutines

To retrieve point property information, use the syntax GET(BANK(XXXX),POS(i)), where "XXXX" is a point property (listed below) and "i" is the order of the component in the GENeral section COMponent command. Use the syntax GET (IBANK(XXX),POS(i)) when the value to be retrieves is an integer or a name.

### Critical point values

ATC	Critical temperature in degrees R.
APC	Critical pressure in PSIA
AVC	Critical volume in FT3/LBMOL.

### Gravities at 60F, 14.696 PSIA.

API	API gravity
SPGR	specific gravity
GPMO	gallons/LBMOL

### Normal boiling point, mole wt.

ATB	mean average boiling point in R, 1 atm.
AMW	molecular weight

### Correlation constants:

ADEL	Solubility parameter in BTU/LBMOL
AOMA	Acentric Factor
WATK	Watson characterization factor (K)
AVW	Characteristic volume in FT3/LBMOLE

### Component id, name:

IDCO Component ID number  
 KOMN (i) Component name. Use KOMN(i) with i=1,2,3,4 to get full name, DO loop recommended

### Inline Fortran: Table 5. Utilities Subroutine (use with CALL)

Type/Name	Description
PTITLE	Causes line printer to skip to top of next page and print Design II page banner and job title.
LINECK(N)	Increases line count by N; starts new page if total count exceeds 55 lines. This should be used any time the WRITE or print statement(s) are used.
COPSTR(i,j)	Copies all information about stream "i" into stream "j", where "i" and "j" are assigned stream numbers.
INISTR(i)	Used to initialize stream "i" after changing parameters with "SET".
RAPSON(N,X,F,DX,TOL,IC)	Solves sets of nonlinear equations.

where

- N = number of equations
- X(N) = independent variables
- F(N) = error functions ( - 0)
- DX = step size as fraction of X(N), about 0.01
- TOL = convergence tolerance
- IC(1) = returns 1 when converged
- IC(2) = 0 to set up new Jacobian (J)
- IC(2) = -1 to start with prior J inverse
- IC(2) = 1 to start with identity matrix
- IC(3) = current iteration number
- IC(4) = current number of J inverse updates

and the following variables have to be dimensioned

DIMENSION X(N), F(N), IC(4)

Non-linear equations which are set up in your ADD BLOCK can be solved using the RAPSON subroutine. This is a modified Newton Raphson technique which provides very rapid convergence.

### Inline Fortran: Table 6. Thermodynamic Library Subroutines (use with CALL)

- KVALUE (XMOL,YMOL,T,P,VK)  
 Calculates K-values given molar compositions for liquid (XMOL), vapor (YMOL) and temperature and pressure.
- VAPENT (YMOL,T,P,HV,SV)  
 Calculates vapor enthalpy and entropy (BTU/LBMOL and BTU/LBMOL/R, respectively).
- VAPRES (I, T, VP)  
 Calculates vapor pressure of pure component. I = Component position i the COMponent list (not the component ID), T = Temperature in degrees Rankine, VP = Vapor pressure in PSIA.
- LIQENT (XMOL,T,P,HL,SL)  
 Calculates liquid enthalpy and entropy.
- DENSTY (WMOL,T,P,NPH,D)\*  
 Calculates actual molar density given the phase molar composition (WMOL). NPH=0 for vapor, NPH=1 for liquid. LBMOL/FT<sup>3</sup>.
- THRCON (IPH,WMOL,T,P,TH)  
 Calculates thermal conductivity given the phase molar composition (WMOL). NPH=1 for vapor, NPH=2 for liquid. BTU/HR/FT/F
- HCAPAC (XMOL, T, P, CP, CV, IPHASE, KEY, JERR)  
 Calculates heat capacity of a mixture. XMOL= Molar composition array (dimension to number of components) , T=Temperature in degrees Rankine, P = Pressure in PSIA, CP = Heat capacity at constant pressure, BTU/lbmol/R, CV= Heat capacity at constant volume, BTU/lbmol/R, IPHASE = 1 for vapor, 2 for liquid, KEY = 0 for Cp and Cv calculation, 2 for Cp calculation only, JERR = 0 for no error occurred, >0 for error flag.
- VISCOS (IPH,WMOL,T,P,VS)  
 Calculates viscosity in centipoise. IPH and WMOL as above.
- SURTEN (XMOL,YMOL,T,P,ST)

## Chapter 18

Calculates surface tension in dynes/cm.

BUBDEW (WMOL,T,P,KEY)\*

Calculates bubble/dew point temperature or pressure. T and P must both be initialized. KEY=1 OR 2 for bubble T (or) dew T calculations, KEY=3 OR 4 for bubble P (or) dew P calculations.

STRCOM(NSTR,FLO,NCP)\*\*

Special subroutine function that retrieves the vector of component flowrates for a specified stream number. Used along with CALL DENSTY routine. NSTR and NCP should be initialized. NSTR -specific stream number, NCP - number of components.

REIDVP (WMOL,RVP,IERR,ERR)

Calculates Reid vapor pressure in PSIA for specified composition. IERR returns zero when converged or 1 otherwise. ERR returns the relative error. Nitrogen must be in the component list.

REICRU (WMOL,RVP,IERR,ERR)

Calculates Reid vapor pressure in PSIA for specified composition. IERR returns zero when converged or 1 otherwise. ERR returns the relative error. Nitrogen must be in the component list.

REIPRO (WMOL,RVP,IERR,ERR)

Calculates Reid vapor pressure in PSIA for specified composition. IERR returns zero when converged or 1 otherwise. ERR returns the relative error. Nitrogen must be in the component list.

\*These routines will use the same thermodynamic property options as the equipment module in which they are called.

\*\*See example [Inline Fortran: Railroad Tank Car Volume Calculation](#).

### Inline Fortran: Table 7. Thermodynamic Interaction Parameters

Binary parameters for WILson, RENon, UNIQUAC, APISOAVE, PENG-Robinson and SOAVE equations can be entered directly in DESIGN II using Inline FORTRAN. The general form of the Inline FORTRAN statement is as follows:

F- SET(BANK(xxxx),POS(ii)) = VALUE

where "xxxx" is a bank name and POS(ii) is the position in the equation matrix (NOT the component ID number or position in the component list).

The equation matrix (column X and row Y) is composed of the binary interaction parameters, and the acentric factors in Column-X1, X2, etc.. and the component to component interactions in Row-Y1, Y2, etc.. This application is very specialized and needs careful incorporation within DESIGN II simulation using Inline Fortran. For additional instructions and procedures for this application, call or fax WinSim Inc.'s DESIGN II Customer Support Group by *Contacting Technical Support*

### Inline Fortran: Activity Coefficient Equations Binary Interaction Parameter

Bank names are **WWIL**, **WREN** and **WUNQ** for the Wilson, Renon and UNIQUAC equations, respectively. Wilson and UNIQUAC equations have a maximum of 4 parameters per binary pair; Renon has 6 parameters. The "B" (temperature dependent) parameters are typically zero.

A three component system yields a 3X3 matrix, in which the diagonals is eliminated. Let's take the system acetone, methanol, and water as an example. If our component list is ordered 1002,1021, 62, then the matrix would look like this:

	<b>1002</b>	<b>1021</b>	<b>62</b>
<b>1002</b>	---	A12	A13
<b>1021</b>	A21	---	A23
<b>62</b>	A31	A32	---

The position numbering begins in column 1 and proceeds downward, then column2, and then column3 (and so forth for systems with more components). Another way to look at this is:

A21  
A31  
A12  
A32  
A13  
A23

### Inline Fortran: Renon Equation Binary Interaction Parameter Data Entry

The Renon equation has 2 "A", 2 "B" and 2 "C" parameters for each binary pair. The position numbering for binary parameters in the bank WREN begins with 5. The "B" parameter positions begin at 5+(NCP(NCP-1)), where NCP is the number of components in the system. The "B" parameters are typically zero. If they are zero, they do not have to be entered. The "C" parameter positions begin at 5+(2NCP(NCP-1)). Although the C12 and C21 parameters are identical you must enter values for both.

Let's enter some values for the "A" parameters into a matrix for the Renon equation using the acetone, methanol, water

system (data from DECHEMA, Vol.1,p.567).

	<b>1002</b>	<b>1021</b>	<b>62</b>
<b>1002</b>	---	2398.5864	340.403
<b>1021</b>	-935.802	---	-169.619
<b>62</b>	2846.293	626.411	---

The matrix for the C parameters would look like this:

	<b>1002</b>	<b>1021</b>	<b>62</b>
<b>1002</b>	---	0.284	0.301
<b>1021</b>	0.284	---	0.309
<b>62</b>	0.301	0.309	---

Using the parameters shown in the sample matrix above, you would add the commands shown in the following example to your standard DESIGN II input file to enter binary parameters for one of the liquid activity coefficient equations (Renon, in this case).

```
MULFLA1=INIT,1,-2
F-      PRE
F-      SET (BANK (WREN), POS (5))=-935.802
F-      SET (BANK (WREN), POS (6))=2846.293
F-      SET (BANK (WREN), POS (7))=2398.5864
F-      SET (BANK (WREN), POS (8))=626.414
F-      SET (BANK (WREN), POS (9))=340.403
F-      SET (BANK (WREN), POS (10))=-169.619
F-      SET (BANK (WREN), POS (17))=0.284
F-      SET (BANK (WREN), POS (18))=0.301
F-      SET (BANK (WREN), POS (19))=0.284
F-      SET (BANK (WREN), POS (20))=0.309
F-      SET (BANK (WREN), POS (21))=0.301
F-      SET (BANK (WREN), POS (22))=0.309
```

```
C- ADD THE REMAINING EQUIPMENT ITEMS..
GEN,
  COM=1002,1021,62
  FLO(LB/HR)1=1000,2000,5000
  TP(F,BAR)1=100,1
  RENON,LAT
END
```

The internal units for the binary parameter bank are BTU/LBMOL. The "C" parameters for the Renon equation are dimensionless and no attempt to convert these should be made.

Use the MULFLA module as the first module in your flowsheet. If you have multiple feed streams to the process, each feed stream must be initialized in the equipment module where the Inline FORTRAN statements for the binary parameters are located. This module should also be the first module calculated.

**Inline Fortran: Wilson Equation Binary Interaction Parameter Data Entry**

The Wilson equation has 2 "A" and 2"B" parameters for each binary pair. The "B" parameters are typically zero. In addition, the Wilson equation includes a molar volume ratio term. The molar volume for each component is also included in the bank WWIL (this is of importance only if you have your own volume data which you prefer to use instead of the pure component data base value). The units for volume are FT3/LBMOL.

The position numbering for the binary parameters in the bank WWIL begins with 5. The "B" parameter positions begin at 5+(NCP\*(NCP-1)). The molar volume position numbering begins at 5+(2\*NCP\*(NCP-1)). If you do not enter the molar volumes, they are automatically retrieved from the data base when the WILSON command is entered.

**Inline Fortran: UNIQUAC Equation Binary Interaction Parameter Data Entry**

The UNIQUAC equation has 2 "A" and 2 "B" parameters, just as the Wilson equation does. This equation also includes molecular area (Q) and volume(R) parameters, plus a Q' parameter for each component in the system. These parameters are automatically supplied from the pure component database for most components (non-condensables and other components for which this information is not available will be supplied with a value of zero).

The Q parameters are stored in the bank WUNQ beginning with position 7, followed by the R parameters and then the Q' parameters. The beginning position for the first UNIQUAC "A" parameter is then 7+3(NCP). The beginning position for the first "B" parameter would be as follows:

$$7 + 3(NCP) + (NCP(NCP-1))$$

**NOTE:** If you do not have interaction parameters for every binary pair in the system, then you do not have to enter zeros for the missing parameters. However, you DO have to assign a position number to the slot for that binary pair when you are numbering the matrix to determine which positions belong to each binary parameter

## Chapter 18

### Inline Fortran: Equations of State Binary Interaction Parameter Data Entry

Bank names are **WSOP**, **WPEN** and **WSOA**, for the API Soave, Peng-Robinson and Soave equations, respectively. Each of these equations has two interaction parameters per binary pair, A and B. The "B" (temperature dependent) parameter is frequently zero. Internal units are BTU/LBMOL. A four component system for an equation of state would yield a 6 X 2 matrix. The columns are the "A" and "B" parameters; the rows are the binary pairs in "component list" order. For GEN, COM =49,46,2,62, the matrix would look like this:

	<u>A</u>	<u>B</u>
<b>49,46</b>	--	--
<b>49,2</b>	--	--
<b>49,62</b>	--	--
<b>46,2</b>	--	--
<b>46,62</b>	--	--
<b>2,62</b>	--	--

The position numbering begins in column 1 and proceeds downward, then column 2 (if any, these are the B parameters). The first binary pair will be numbered  $(6 \times \text{NCP}) + 2$ , where NCP is the number of components. For a 4 component system, this would be position 26. The B parameters begin at  $(6 \times \text{NCP}) + 2 + (\text{NCP}(\text{NCP}-1)/2)$ . Acentric factors (normally from the DESIGN II PURE COMPONENT DATABASE) reside in the third set of NCP-long positions. If you enter your own acentric factors, they should begin at position  $(2 \times \text{NCP}) + 2$ .

### Inline Fortran: PENG-Robinson Equation of State Binary Interaction Parameter Data Entry

Let's enter the results of solubility data regression for CO<sub>2</sub> and N<sub>2</sub> in water to the Peng-Robinson equation. The remainder of the interaction parameters will be supplied from the binary parameter library, PENG1, which resides in DESIGN II. For example, if we have the following parameters,

	<u>A</u>	<u>B</u>
<b>49,46</b>		
<b>49,2</b>		
<b>49,62</b>	-.18438	.11948e-3
<b>46,2</b>		
<b>46,62</b>	-.1163	.1035e-2
<b>2,62</b>		

Enter the following commands in our DESIGN II input file or the Inline Fortran template of the equipment module.

```
FLA1 = SEP, 1, -2, -3
F-     PRE
F-     SET (BANK (WPEN) , POS (28) ) = -.18438
F-     SET (BANK (WPEN) , POS (30) ) = -.1163
F-     SET (BANK (WPEN) , POS (34) ) = .11948E-3
F-     SET (BANK (WPEN) , POS (36) ) = .1035E-2
..
..
rest of equipment data
..
..
..
GENeral,
  COM=49,46,2,62
  FLO (LB/HR) 1=1000,2000,5000
  TP (F,BAR) 1=100,1
  PENK, PENH, STDD,
  BIN PAR=PENG1
..
..
rest of flowsheet data
..
..
END
```

### Inline Fortran: BWR and BWRS Equation of State Binary Interaction Parameter Data Entry

Bank names for the BWR equations are BWR and BWRS, corresponding to the DESIGN II K-value options BWRK and BWRSK. Each of these equations has one interaction parameter per binary pair and eleven pure component constants. They are illustrated in the Table below:

You can add the pure component constants and one binary interaction parameter per component pair for components which are not included in the Table. Details for using Inline FORTRAN are shown on the following sections.

#### Table for BWR and BWRS Components

<u>BWR Components</u>	<u>ID No.</u>	<u>BWRS Components</u>
-----------------------	---------------	------------------------

methane	2	methane
ethane	3	ethane
propane	4	propane
i-butane	5	i-butane
n-butane	6	n-butane
i-pentane	7	i-pentane
n-pentane	8	n-pentane
nitrogen	46	nitrogen
carbon dioxide	49	carbon dioxide
	50	hydrogen sulfide
	22	ethylene
	23	propylene
	10	hexane
	11	heptane
	12	octane
	13	nonane
	14	decane
	15	undecane

**BWR and BWRs Pure Component Constants**

There are eleven pure component parameters for the BWR equations. They are stored in the following order, beginning in position 6 of either BANK BWR or BWRs:

Bo1	through	Bon
Ao1**1/2	through	Aon**1/2
Co1**1/2	through	Con**1/2
Do1**1/2	through	Aon**1/2
Eo1**1/2	through	Aon**1/2
ao1**1/3	through	aon**1/3
bo1**1/3	through	bon**1/3
co1**1/3	through	con**1/3
do1**1/3	through	don**1/3
o1**1/2	through	on**1/2
o1**1/3	through	on**1/3

The 1 and n are the first through the last components in COMponent list order. The 1/2 and 1/3's in the above constants refer to square root and cube root, respectively. See page 221 of Kenneth E. Starling's book, Fluid Thermodynamic Properties for Light Petroleum Systems. (Gulf Publishing Co., Houston, 1973), for the equations to use to compute these pure component constants. Units for critical density are LBMOL/FT3 and degrees R for critical temperature.

**BWR and BWRs Binary Interaction Parameters(Kij)**

The BWR equations allow one Interaction parameter per binary pair. The value you enter for the binary interaction parameter is (1-Kij) and it is in BTU/LBMOL. A four component system for the BWR equations yields a 4 by 4 matrix. Both the columns and the rows are labeled with binary pairs in COMponent list order. e.g. For COM=2,1,23,3, the form of the matrix is:

	<b>2</b>	<b>1</b>	<b>23</b>	<b>3</b>
<b>2</b>	K2,2	K1,2	K23,2	K3,2
<b>1</b>	K2,1	K1,1	K23,1	K3,1
<b>23</b>	K2,23	K1,23	K23,23	K3,23
<b>3</b>	K2,3	K1,3	K23,3	K3,3

Positions are counted beginning in the column 1 and proceeding downward, then column 2, etc. Although Kij=Kji and Kii and Kjj=0, you must enter all binary parameters in the matrix (for component pairs not in Table 1) whether they are zero or not. Since the value you are entering is actually (1-Kij), you should enter a value of 1.00 for all Kii and Kjj parameters. The position numbering for binary interaction parameters begins with 6 + (15\*NCP).

Let's add the Bo and Ao constants for hydrogen (using a Tc of -375 F as recommended by Starling for calculations above 0 F) and the methane-ethylene interaction parameter. They are 0.35535 (Bo), 30.5753(Ao) and 0.979 (Kij). We would enter the following commands in our DESIGN II input file using Inline FORTRAN:

```
FLA1 = SEP, 1, -2, -3
F-     PRE
F-     SET (BANK (BWRs) , POS (7) ) = .35535
F-     SET (BANK (BWRs) , POS (10) ) = 30.5753
F-     SET (BANK (BWRs) , POS (68) ) = .0.979
F-     SET (BANK (BWRs) , POS (74) ) = 0.979
..
..
rest of equipment data
..
..
```

## Chapter 18

```

..
GENeral,
  COM=2,1,23,3
  FLO(LB/HR)1=100,200,500,750
  TP(F,BAR)1=100,1
  BWRSK, BWRSH, BWRSD,
..
..
rest of flowsheet data
..
..
END

```

### Inline Fortran: Table 8. DESIGN II Flash Subroutine (use with CALL)

It is possible to CALL the DESIGN II flash routine, FLASH1, to perform adiabatic or isothermal flashes on a stream and separate it into 1, 2, or 3 phases. All information about the flashed stream and the resulting phases is passed through the argument list as follows:

```

      CALL FLASH1 (NIN, NPH, NCP, NPAR1, NPAR2,
1         DUMMY1, TIN, PIN, HIN, FIN, XIN, DUMMY2,
2         VFOUT, TOUT, POUT, HOUT, FOUT, XOUT,
3         AKOUT, DECANT, PAR1, PAR2)

```

For an isothermal flash set PAR1(2)=1., and also set TIN, PIN, FIN, and XIN. For an adiabatic flash set PAR1(2)=2., and also set PIN, HIN, FIN, and XIN. For an adiabatic flash set PAR2(4) equal to the heat added to or subtracted from the flash. A negative value indicates heat subtracted.

The FLASH1 routine flashes one stream and separates it into 1, 2 or 3 streams depending on the value of NPH ("number of phases"). The figure below illustrates the flow of information to and from the FLASH1 routine.

Input Arguments	Output Arguments
TIN, PIN, etc.	TOUT(1), POUT(1), etc.
	TOUT(2), POUT(2), etc.
	TOUT(3), POUT(3), etc.

If NPH=1, then there is no phase separation and the stream results are all in the first outlet stream variables: TOUT(1), POUT(1), HOUT(1), etc. The flowrate of any immiscible water is also calculated and placed in DECANT(1).

If NPH=2, then the vapor phase is placed in the first outlet and the total liquid phase in the second. The flowrate of any immiscible water is also calculated and placed in DECANT(2).

If NPH=3, then the vapor phase is placed in the first outlet, liquid hydrocarbon in the second outlet (including any soluble water), and the free water phase in the third outlet (including any soluble hydrocarbons). IMM=62 must be set in the GENERAL section. The variable DECANT is not used in this case for the immiscible water flowrate.

A complete description of the variables passed to and from the FLASH1 routine is given below:

#### Input

Arguments	Meaning
NIN	(scalar), Must be set = 1
NPH	(scalar), Number of separate outlet streams: 1, 2, or 3.
NCP	(scalar), Number of components
NPAR1	(scalar), Length of PAR1 vector
NPAR2	(scalar), Length of PAR2 vector
DUMMY1	(scalar), Not used but must be in argument list
TIN	(scalar), Temperature of inlet stream in R
PIN	(scalar), Pressure of inlet stream in PSIA
HIN	(scalar), Enthalpy of inlet stream in BTU/HR
FIN	(scalar), Total molar flowrate of inlet stream in LBMOL/HR
XIN	(matrix, NCP by NIN), Component flowrates of inlet stream (LBMOL/HR)
DUMMY2	(matrix, NCP by NIN), Not used but must be in argument list
PAR1	(vector, length of at least 5), PAR1(2)=1 for isothermal flash, PAR1(2)=2 for adiabatic flash
PAR2	(vector, length of at least 5), PAR2(4)= heat added to or subtracted from HIN for adiabatic flash, otherwise set to zero. Negative indicates heat subtracted.

#### Output

Arguments	Meaning
VFOUT	(vector, length NPH), Vapor fractions of outlet streams
TOUT	(vector, length NPH), Temperatures of outlet streams in R
POUT	(vector, length NPH), Pressures of outlet streams in PSIA
HOUT	(vector, length NPH), Enthalpies of outlet streams in BTU/HR



<b>FOUT</b>	(vector, length NPH), Total molar flows of outlet streams in LBMOL/HR
<b>XOUT</b>	(matrix, NCP by NPH), Component flowrates of outlet streams (LBMOL/HR)
<b>AKOUT</b>	(matrix, NCP by NPH), K-values of outlet streams
<b>DECANT</b>	(vector, length NPH), Flowrate of immiscible water in LBMOL/HR is placed in the one element DECANT(NPH). Used only if IMM=62 is set in GENERAL section. For example if NPH=2, then there are 2 outlet streams and DECANT(2) is set to the flowrate of immiscible water. The immiscible water in DECANT is 100% pure whereas the more rigorously calculated third output stream contains immiscible water plus soluble hydrocarbons.

## Inline Fortran: Table 9. REFIne Module Subroutines

### Use with CALL:

#### REFLIQ (X,ITRAY,IFLAG)

Retrieves the liquid compositions on each tray of the REFIne column. These commands must appear in the REFIne module to which they pertain. ITRAY = tray for which the liquid or vapor composition is desired. Trays are numbered from top to bottom with the condenser as tray 0. X/Y = composition of the liquid/vapor. X and Y must be dimensioned equal to the number of components in the component list. IFLAG = 1 for mole fractions, 2 for mass fractions.

#### REFVAP (Y,ITRAY,IFLAG)

Retrieves the vapor compositions on each tray of the REFIne column. These commands must appear in the REFIne module to which they pertain. ITRAY = tray for which the liquid or vapor composition is desired. Trays are numbered from top to bottom with the condenser as tray 0. X/Y = composition of the liquid/vapor. X and Y must be dimensioned equal to the number of components in the component list. IFLAG = 1 for mole fractions, 2 for mass fractions.



# Chapter 19: Interactive Processing

## Interactive Processing Overview

Interactive Processing is a useful DESIGN II feature which is available as an option on some computer systems. It allows modification and review of equipment and stream data while DESIGN II is executing. Time and money can be saved using this feature by minimizing reruns. To use interactive processing, simply add an **INTERACTIVE ON** command to almost any equipment module to review results or change specifications dynamically.

During execution of DESIGN II, the program will stop and wait for interactive commands for each equipment selected to be processed interactively. Simply choose items to review or modify before allowing the program to continue. The first time a menu appears for an equipment module, the unit has not been calculated. Certain printing commands can be executed during interactive processing that allow comparison of results as parameters are changed.

The following list shows which DESIGN II modules are/are not available to interactive processing.

<b>Available</b>	<b>NOT Available</b>
Component Splitter	Continuous Stirred Tank Reactor
CompressorController	
Distillation	Depressuring
Divider	Equilibrium Reactor
Expander	Fired Heater
Flash	Flow Meter
Heat Exchanger	Hydrotreater
LNG Exchanger	Line Pressure Drop
Mixer	Multiphase Flash
Multiple Flash	Phase Envelope
Polytropic Compressor	Phase Map
Pump	Plug Flow Reactor
Reactor	Refine Column
Shortcut Distillation	Add Block
Stream Manipulator	Amine Column
Valve	

**NOTE:** The Inline FORTRAN features "DISPLAY" and "INPUT" are not available when in the INTERACTIVE mode.

## Interactive Processing Command Details

### **INTERACTIVE ON**

To activate the interactive processing capability, add this command to the desired equipment module in the simulation run. Once in the interactive mode, five associated menus become active:

#### **COM**mands

Controls selection of the equipment parameters to be monitored.

#### **ST**ream

Displays current detailed stream information.

#### **UN**its

Allows the user to change the units of the interactive display on the screen.

#### **CON**trols

Controls printing and calculation options.

#### **EQU**ipment

Allows modification and monitoring of equipment parameters before and after equipment execution.

Any of the above menus are accessible from within any other menu.

The COMmands menu only appears for the first of each equipment type. To change a list of displayed commands for an equipment module, simply type COM and the COMmands menu will appear.

The example in the next section demonstrates the use of the menus in an interactive session. However, the UNIts menu and the simple scroll command are not demonstrated and therefore are discussed below.

## Interactive Processing Units Menu

DESIGN II uses default units (American units) for the equipment commands displayed. These units can easily be changed via

## Chapter 19

the UNITS menu. Once a unit of a given type (e.g. pressure, temperature) has been changed using the UNITS menu, it will remain the same until you change it again. The UNITS menu and the possible unit option for each unit type are shown below:

```
UNITS MENU
1 -   pressure unit
2 -   temperature unit
3 -   area unit
4 -   length unit
5 -   heat unit
6 -   time unit
7 -   molar Q units
8 -   mass Q units
9 -   quantity units
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus   : (STR)EAM, (COM)MANDS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
```

### Dimensional Unit Options

```
ENTER: Number of pressure unit
      1-PSIA 2-ATM 3-MMHG
      4-BAR 5-KG/CM2 6-KG/M2
      7-DY/CM2 8-G/CM2 9-PA
      10-KPA 11-PSIG
ENTER: Number of temperature unit
      1-F 2-C 3-R
      4-K
ENTER: Number of area unit
      1-FT2 2-CM2 3-M2
      4-MM2 5-YD2 6-IN2
ENTER: Number of length unit
      1-FT 2-CM 3-M
      4-MM 5-YD 6-IN
      7-MILE 8-KM
ENTER: Number of heat unit
      1-BTU 2-CAL 3-KCAL
      4-FTLB 5-J 6-KJ
      7-MAJ
ENTER: Number of time unit
      1-HR 2-SEC 3-MIN
      4-DAY 5-YR
ENTER: Number of molar Q units
      1-LBMOL 2-GMOL 3-KGMOL
ENTER: Number of mass Q units
      1-LB 2-G 3-KG
      4-TON 5-TONNE
ENTER: Number of quantity units
      1-LBMOL 2-GMOL 3-KGMOL
      4-LB 5-G 6-KG
      7-TON 8-TONNE 9-GAL
      10-BBL 11-LIT 12-M3LIQ
      13-FT3 14-SCF 15-MSCF
      16-MMSCF 17-M3API 18-M3VAP
```

Input units for individual equipment commands can also be changed by typing "C" for change instead of the new value when in the EQUIPMENT menu. This has no effect on the display or output units.

## Interactive Processing Scroll Commands

The COMMANd and EQUIPMENT menus may contain more equipment parameters (command) numbers than can be displayed on a single screen. This may also occur for STREAM data from the STREAM menu. When this occurs, the menu will contain the following message:

```
Scroll commands:
(U)P, (D)OWN, (T)OP, or (B)OTTOM
```

The (U)p and (D)own commands scroll the display a specified number of lines; thus the U and D commands can be followed by a number. For example, to move down 16 lines (a full screen),

### Type: D16

Menu lines 17 through 32 are then displayed. If there were fewer than 32 commands, the last 16 lines would be displayed. The (T)op and (B)ottom commands display the top or bottom 16 lines, respectively.

## Interactive Processing Example

(From the DESIGN II Menu Bar, please select...File...Open...c:\designii\samples\interact\interac.psd to simulate this  
302 DESIGN II General Reference Guide

## problem)

Here is a simple example that shows some typical interactive prompts and responses. The input below consists of a FLAsh with a heat change, followed by an EXPander unit. One object of this problem is to remove enough heat from the flash drum inlet stream, 16, to recover 60% of the ethane (or 1.2 lbmol/hr) in the liquids. This is accomplished by interactively adjusting the heat removed from stream 16. The INTERACTIVE ON command is added to the FLAsh module. The initial guess for heat removed is 35500 Btu/hr.

**NOTE:** In the following text "(CR)" is the symbol for pressing the carriage return key. Since all input commands require a (CR) in order to be executed, the (CR) is implied and not shown.

## Coding

```

AB123.
*EXPANDER PLANT
FLAsh 19 = S306, 16, -11,-44,
      HEAt = -35500, ADIabatic
      INTERACTIVE ON,
EXPander 37 = E33, 11, -31, -33
      PREssure OUT = 300
GENeral
COMPonents = 2,3,4, FLOW 16 = 10,2,1
      TP 16 = 100,800
      KVAL, COPE
END
  
```

After submitting the job for execution, the following information appears on the screen:

```

NOW PROCESSING INPUT                      13:43:18
NOW PROCESSING PURE COMPONENT DATA       13:43:25
NOW PROCESSING STREAM INITIALIZATION
13:43:28 FLAsh      EQ NO. = 19 NAME = U30
  1          HEAt
  2          TEMperature of EXChange
  3          TEMperature OUT
  4          PREssure OUT
  5          BUBBle point
  6          DEW point
  7          DEW WATER
  8          ISOthermal
  9          ADIabatic
 10          ISEntropic
 11          LIQuid
 12          VAPor
 13          LIQuid FRAction
 14          WATER ENTrained in OIL
 15          OIL ENTrained in WATER
 16          KKEY
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus: (STR)EAM, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
  
```

The program executes up to the FLAsh module and then stops, because of the INTERACTIVE ON command. The FLAsh module and parameters are listed so that the desired information to be displayed or changed can be selected. To select display of the HEAt command:

## Type: 1

```

FLAsh      EQ NO. = 19 NAME = 5306
1          *HEAt
2          TEMperature of EXChange
3          TEMperature OUT
4          PREssure OUT
5          BUBBle point
6          DEW point
7          DEW WATER
8          ISOthermal
9          ADIabatic
10         ISEntropic
11         LIQuid
12         VAPor
13         LIQuid FRAction
14         WATER ENTrained in OIL
15         OIL ENTrained in WATER
16         KKEY
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus : (STR)EAM, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
An * appears beside HEAt to show that this parameter has been selected to display. Now select the
(CON)TROLS Menu to continue the run.
  
```

# Chapter 19

## Type: CON

```
CONTROLS MENU
  1 - Redo calculation
  2 - Print column profile
  3 - Print recycle sequence
  4 - Continue
  5 - Quit
Other Menus : (STR)EAM, (COM)MANDS, (UNI)TS or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
```

Remember, the first time a menu appears for an equipment module, the module has not been calculated. Therefore, select the option to execute the FLAsh calculation. (If "4-Continue" is chosen, the program will run to completion or to the next interactive equipment.)

## Type: 1

```
NOW CALLING EQUIPMENT 19 + FLA = S306 13:43:52
FLAsh EQ NO. = 19 NAME = S306
  1 HEAT (BTU/HR) = -35500.
Other Menus: (STR)EAM, (COM)MANDS, (UNI)TS or (CON)TROLS
ENTER: Number (from menu) or Another MENU
```

## Type: STR

```
DESIGN II has now executed the FLAsh module using the initial guess of 35500 Btu/hr heat removed.
  Select the (STR)eam Menu to see the amount of ethane recovered in the initial flash calculation.
STREAM MENU
  1 - Stream Data
  2 - Stream Properties
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
```

## Type: 1

```
Streams in      16
Streams out     11      44
Enter stream number
```

**NOTE:** Any stream number in the simulation can be reviewed. Only the numbers of the streams which are associated with the current module will be listed. Streams which are not feed streams or have not been calculated will show zero flows and properties.

## Type: 44

```
Stream Number: 44      Flow Rates      /HR
Temperature (F)      -39.067      Pressure (PSIA)      800.000
Enthalpy (BTU/HR)    -20568.      Vapor Fraction      0.0000
Component Name      TOTAL      LIQUID      VAPOR      TOTAL      TOTAL
                   LBMOL      LBMOL      LBMOL      LB      MOL PCT KVALUE
-----
METHANE             2.362      2.362      0.000      37.894      55.188
ETHANE              1.139      1.139      0.000      34.236      26.604
PROPANE             0.779      0.779      0.000      34.363      18.209
-----
TOTAL               4.280      4.280      0.000      106.5      100.000
  ENTER (SAV)E to save screen to output file or
  Press enter to return to STREAM MENU
```

Only 1.14 lbmol/hr of ethane were recovered in the liquids; therefore, increase the heat removed from feed stream 16. To get back to the (STR)eam Menu,

## Type: (CR)

```
STREAM MENU
  1 - Stream Data
  2 - Stream Properties
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll
  Command or Another Menu
Select (EQU)IPMENT Menu to change the heat removed.
```

## Type: EQU

```
FLAsh EQ NO. = 19 NAME = S306
  1 HEAT (BTU/HR) = -35500.
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
```

## Type: 1

```
ENTER: HEAT in BTU/HR
  or (C)HANGE to change units
```

**Type: -36500**

```

          FLash      EQ NO. = 19 NAME = S30
    1 HEat (BTU/HR) = -36500.
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll
             Command or Another Menu
    
```

Now rerun the flash calculation by selecting the (CON)TROLS Menu and repeating the flash calculation.

**Type: CON**

```

CONTROLS MENU
1 - Redo calculation
2 - Print column profile
3 - Print recycle sequence
4 - Continue
5 - Quit
Other Menus : (STR)EAM, (COM)MANDS, (UNI)TS or (EQU)IPMENT ENTER: Number (from menu), Scroll Command
             or Another Menu
    
```

**Type: 1**

```

NOW CALLING EQUIPMENT      19  +   FLA      =   S306      14:00:23  + FLash      EQ NO. = 19
          NAME = S30
    1 HEat (BTU/HR) = -36500.
Other Menus: (STR)EAM, (COM)MANDS, (UNI)TS or (CON)TROLS
ENTER: Number (from menu) or Another MENU
    
```

**Type: STR**

```

STREAM MENU
1 - Stream Data
2 - Stream Properties
Scroll Commands: (U)P, (D)OWN, (T)OP, or (B)OTTOM
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll
             Command or Another Menu
    
```

**Type: 1**

```

Streams in      16
Streams out     11      44
Enter stream number
    
```

**Type: 44**

```

Stream Number:  44      Flow Rates      /HR
Temperature (F) -41.399  Pressure (PSIA)      800.000
Enthalpy (BTU/HR) -21805.  Vapor Fraction      0.0000
    
```

Component Name	TOTAL LBMOL	LIQUID LBMOL	VAPOR LBMOL	TOTAL LB	TOTAL MOL PCT	KVALUE
METHANE	2.569	2.569	0.000	41.214	56.341	
ETHANE	1.193	1.193	0.000	35.871	26.164	
PROPANE	0.798	0.798	0.000	35.175	17.495	
TOTAL	4.560	4.560	0.000	112.3	100.000	

```

ENTER (SAV)E to save screen to output file or
Press enter to return to STREAM MENU
    
```

The results show that 1.19 lbmol/hr of ethane were recovered. Increase the heat removed one more time in order to recover at least 1.2 lbmol/hr.

**Type: (CR)**

```

STREAM MENU
1 - Stream Data
2 - Stream Properties
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll
             Command or Another Menu
    
```

**Type: EQU**

```

          FLash      EQ NO. = 19 NAME = S30
    1 HEat (BTU/HR) = -36500.
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
ENTER: Number (from menu), Scroll Command or Another Menu
    
```

**Type: 1**

```

ENTER: HEat in BTU/HR
or (C)HANGE to change units
    
```

**Type: -37000**

```

          FLash      EQ NO. = 19 NAME = S306
    1 HEat (BTU/HR) = -37000.
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT
    
```

# Chapter 19

ENTER: Number (from menu), Scroll Command or Another Menu

## Type: CON

CONTROLS MENU  
1 - Redo calculation  
2 - Print column profile  
3 - Print recycle sequence  
4 - Continue  
5 - Quit  
Other Menus : (STR)EAM, (COM)MANDS, (UNI)TS or (EQU)IPMENT  
ENTER: Number (from menu), Scroll Command or Another Menu

## Type: 1

NOW CALLING EQUIPMENT 19 + FLA = S306 14:03:59  
+ FLAsh EQ NO. = 19 NAME = S30  
1 HEAT (BTU/HR) = -37000.  
Other Menus: (STR)EAM, (COM)MANDS, (UNI)TS or (CON)TROLS  
ENTER: Number (from menu) or Another MENU

## Type: STR

STREAM MENU  
1 - Stream Data  
2 - Stream Properties  
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll Command or Another Menu

## Type: 1

Streams in 16  
Streams out 11 44  
Enter stream number

## Type: 44

Stream Number: 44 Flow Rates /HR  
Temperature (F) -42.529 Pressure (PSIA) 800.000  
Enthalpy (BTU/HR) -22444. Vapor Fraction 0.0000

Component Name	TOTAL LBMOL	LIQUID LBMOL	VAPOR LBMOL	TOTAL LB	TOTAL MOL PCT	KVALUE
METHANE	2.680	2.680	0.000	42.993	56.937	
ETHANE	1.220	1.220	0.000	36.689	25.925	
PROPANE	0.807	0.807	0.000	35.567	17.138	
TOTAL	4.707	4.707	0.000	115.2	100.000	

ENTER (SAV)E to save screen to output file or  
Press enter to return to STREAM MENU

1.22 lbmol/hr of ethane were recovered: therefore, complete the simulation by executing the EXPander calculation

## Type: (CR)

STREAM MENU  
1 - Stream Data  
2 - Stream Properties  
Other Menus : (COM)ANDS, (UNI)TS, (CON)TROLS, or (EQU)IPMENT ENTER: Number (from menu), Scroll Command or Another Menu

## Type: CON

CONTROLS MENU  
1 - Redo calculation  
2 - Print column profile  
3 - Print recycle sequence  
4 - Continue  
5 - Quit  
Other Menus : (STR)EAM, (COM)MANDS, (UNI)TS or (EQU)IPMENT ENTER: Number (from menu), Scroll Command or Another Menu Select option 4 to complete the simulation.

## Type: 4

NOW CALLING EQUIPMENT 37 + EXP = E33 14:05:14  
NOW CALCULATING STREAM PROPERTIES 14:05:17  
NOW PROCESSING STREAM PRINT 14:05:18  
NOW PROCESSING EQUIPMENT PRINT 14:05:19  
NOW PROCESSING DETAILED STREAM PRINT 14:05:20  
\*\*\* END OF SIMULATION \*\*\*

By executing this problem interactively, the EXPander module was only called once rather than three times; thus, computer time and CCU charges were reduced. Also, the inherent time between runs (i.e. generation and review of printout, etc.) was saved.



**NOTE:** The Stream Data and Stream Properties screens contain an option to save the screen information (see above). If this option is selected, the screen information will be printed in the output file in the "NOW CALLING" section for each module where interactive results are saved. In this way, a permanent record of the interactive progression can be generated.



# Chapter 20: Size Lines

## Size Lines Overview

Sizing calculations can be requested for any of the lines (streams) in your flowsheet simply by adding a few extra commands in your input file. For example you can size reboiler return lines having two phase flow by coding the reboiler as a heat exchanger and sizing its outlet stream or using internal streams for the DiStillation column. Both single and two-phase lines can be sized to meet specifications of pressure drop, velocity, sonic velocity fraction, or nominal diameter.

The line sizing commands are entered in special Sizing Lines Sections, similar to the GENeral Section, each of which starts with the command:

### SIZE LINES

All commands following this are interpreted as line sizing commands until the next equipment module identifier, GENeral command, END, or another SIZE LINES section is encountered. Lines may be sized using different specifications by coding them in different SIZing LINE Sections. Essentially no limit on the number of these sections in the run exist.

The calculation methods used are mainly applicable to hydrocarbon systems in small diameter lines, and results will vary with the density and viscosity correlations used in your simulation. The correlations for two-phase flow are largely empirical and their accuracy varies considerably, even within the range of the correlated data. Use of these methods for situations other than those intended by the authors is not recommended.

If you are sizing a long transmission line with elevation effects, intermediate compression, or heat transfer, then you should use the LINE module instead of the SIZE LINES section.

Physical properties of the fluid are obtained automatically from DESIGN II inlet stream information and do not have to be entered. These correspond to line inlet conditions only, not average or outlet conditions.

The thermodynamic options you choose in the GENeral section will be used to generate K-values and enthalpies. For heat and material balance calculations, the K-values and enthalpies are the most critical properties. For calculating pressure drops in lines other physical properties, particularly density and viscosity, are also important. Some guidelines for density choices follow:

### COPED

Can be used for natural gas mixtures up to about 400F if the mixture does not contain large amounts of CO<sub>2</sub> or H<sub>2</sub>S.

### BWRSD

Can be used for most hydrocarbon and inorganic gases at high pressures.

### STDD

Can be used for most other systems, including mixtures such as methanol and water.

**NOTE:** Both COPED and BWRSD are based on density data and can be slow in execution.

The program gives you a choice of 3 available pipe sizes with flow details for each. The one labeled "TARGET" is the smallest size which satisfies the user specification. One size larger and one size smaller are also calculated. The size smaller will exceed the specification but may be close enough to be useful. The larger size will provide a smaller pressure drop and offer lower velocity. For two-phase horizontal flow, the Baker flow regime is also given showing the location of all three sizes which were calculated.

Pressure drop in a line is considered due to the effects of friction and of elevation. Any pressure drop due to acceleration is ignored since it is usually insignificant. Details of the methods used for friction and elevation are given.

Sonic velocity in the gas phase is estimated using the generalized correlation of T. K. Sherwood (Reference 8). Each line is checked to make sure that the flow is subsonic. Sonic velocity is also reported.

The default viscosity option is NBS81 (Ely-Hanley, National Bureau of Standards). It is the best correlation available for predicting low molecular weight hydrocarbon vapor and liquid viscosities. The DEAN and Stiel technique was developed for estimating vapor viscosities. It is generally poor for estimating liquid viscosities and should not be used for SIZE LINE calculations for liquid or two-phase lines. The API technique is the default viscosity option when your input includes CRUde, REFIne, or PETroleum STReams commands. If the feed contains significant amounts of light components (methane through pentanes, CO<sub>2</sub>, H<sub>2</sub>S and N<sub>2</sub>), you may want to use the NBS81 option instead. Simply enter either of the following commands in the GENeral section:

**TRANS = NBS81**            or            **VIS = NBS81.**

### Calculation Method

Several options are available for calculating pressure drop. Phase (gas, liquid, or two-phase), direction of flow, and flow regime determine which calculation options are suitable. If you do not specify any of the options, the program has a default set selected according to the phase and direction of flow (See *Line: Default Methods of Calculation Table*). If you choose an inappropriate method for the predicted phase, flow regime, or direction of flow

DESIGN II will print a warning message and switch to the default calculation option(s). Lines which are almost all vapor (at

## Chapter 20

---

vapor fraction .999 and above), and lines which are almost all liquid (at vapor fraction .001 and below) are automatically calculated as single phase.

### Size Lines Command Details

---

#### Size Lines: Required Commands

---

##### SIZE LINES

The line sizing commands are entered in special Sizing Lines sections, similar to the GENERAL Section, each of which begins with the SIZE LINE command.

##### USE streams =

Enter the stream numbers of the lines which are to be sized in this section. This command should be the first command following SIZE LINES.

---

#### Size Lines: Sizing Criteria Commands

---

(enter **only ONE** of the following commands)

##### MAXimum DELta P per hundred feet (P units) =

Enter the maximum allowable pressure drops for each of the streams in the USE streams command. Default value is 0.5 PSI per hundred feet.

##### MAXimum VELOCITY (L units/t units) =

Enter the maximum allowable velocities for each of the streams in the USE streams command. Velocity is calculated at inlet conditions. Normally units should be specified since the default units are FT/HR *not* FT/SEC.

##### NOMinal DIAMeter (L units) =

Enter the nominal diameters of each of the lines to be calculated. See *Line: Nominal Pipe Diameter Table*.

##### MAXimum SONic fraction =

Enter the maximum allowable fractions of sonic velocity for each of the lines on the USE streams command. Sonic velocity is calculated at inlet conditions.

---

### Size Lines Optional Command Details

---

#### Size Lines: Pipe Geometry Specification

---

##### INSide DIAMeter (L units) =

Enter the inside diameters of each of the lines on the USE streams command. The default value is determined from the nominal diameter and the pipe table (*Line: Nominal Pipe Diameter Table*).

##### PIPe WALl code =

Enter the desired pipe wall thickness code. Available options are **STD**, **XS** and **XXS**, which indicate Standard, Extra Strong, and Double Extra Strong wall respectively. STD is the default.

##### LENGth of pipe (L units) =

Enter the length of the pipe for each line in the USE streams command. Default is 100 feet.

##### EQUivalent length (L units) =

Enter the equivalent lengths of bends and fittings for each line on the USE streams command. These values will be added to the actual length for calculations. Default is zero.

##### DIRection of flow =

Enter the direction of flow for each of the lines on the USE streams command. Default is **HOR**izontal. Other possible directions are **UP** or **DOWN**.

##### ELEvation of pipe (L units) =

Enter the elevation of the pipe for each of the lines on the USE streams command. Values entered should be positive for upwards inclined flow and negative for downwards inclined flow. Default value is zero for **HOR**izontal pipe, length of pipe for **UP**wards flow, and negative pipe length for **DOWN**wards flow.

---

#### Size Lines: Pipeline Transport Efficiency

---

##### ROUghness (L units) =

Enter the absolute pipe wall roughness for each of the lines on the USE streams command. *Line: Typical Absolute Surface Roughness Values Table* lists some typical absolute roughness values. Default value is 0.00015 feet which represents commercial steel pipe in normal service. *Line: Nominal Pipe Diameter Table* shows the nominal diameter for given pipe code.

##### DRAg factor =

Enter the appropriate fraction for use in the AGA equation. This should be entered whenever **MET FRI = AGA** is used.

---

One value should be entered for each line specified in the USE streams command. The default value is 1.0 but the user should normally supply a value in the range .9 to .985 (Figure 1.). The drag factor is used to determine the transition Reynolds number and to predict the AGA friction factor when flow is partially turbulent.

pipeline **EFF**iciency = (fraction)

Enter the fractional pipeline efficiency for use primarily in the Panhandle A and Modified Panhandle equations. It can also be applied to the Weymouth equation if desired. Default is 1. *Line: Typical Pipeline Efficiency Values Table* gives some typical values. One value should be entered for each line specified in the USE streams command.

---

### Size Lines: Pipeline Phase Specification

---

**SET** phase of calculation =

Enter the phase (LIQ or VAP) for each line on the USE streams command you want to be calculated as single phase. The default is the phase as determined by the program. This command is only needed if you want to force the program to treat a two-phase line as single phase when the stream is almost all liquid or vapor (within 10 percent on a molar basis). At larger percentages this command is ignored and two phase calculations are performed.

---

### Size Lines: Pressure Drop Calculation Method

---

All of the gas methods can be used to size wet gas lines with some liquid provided that the vapor fraction is 0.9 or over. Below this vapor fraction the program considers gas methods inappropriate and changes to the default method for two-phase calculations. See *Line: Default Methods of Calculation Table*

**METH**od for **FRI**ction pressure drop =

Enter one of the options for calculation of pressure drop due to friction for each line on the USE streams command. The default method is dependent on phase and direction of flow.

**AGA**

Equation for friction pressure drop (and also elevation pressure drop) calculated by the general flow equation. This is for both fully and partially turbulent gas flow. The American Gas Association elevation pressure drop method is automatically used with it unless a different method for elevation is specified. DRAG factor, which is normally in the range .9 to .985, should be specified whenever MET FRI = AGA is used.

**BEG**gs and Brill

The Beggs and Brill correlation is an integrated method for pressure drop calculation for two phase systems. With specification of BEGs as the friction pressure drop method all other calculation methods for elevation effects, friction factor, flow regime, and holdup default to the Beggs and Brill technique automatically. (Reference 18)

**DAR**cy-Weisbach

Default equation for single phase flow, suitable for all flow regimes where calculated pressure drop is under ten percent of the inlet pressure (Reference 9). It is least accurate in the transition zone from partially to fully turbulent flow.

**DUK**ler

The DUKler correlations for two-phase pressure drop use the constant slip (Case II) method. (Reference 17) Unless you specify otherwise, the DUKler method for friction factor will also be used.

**DUN**s Ros.

Duns-Ros is used for two phase flow in vertical pipes. Duns-Ros flow regime and holdup methods are used automatically when this option is selected for friction pressure drop, unless you choose an alternate holdup method. (Reference 13)

**HAG**edorn Brown

Hagedorn Brown is used for two phase flow in vertical pipes. (Reference 24)

**LOCK**hart-Martinelli

Default equation for calculating pressure drop due to friction in two-phase, horizontal lines. The method is implemented as described by Kern (Reference 2) using the Baker flow regime map. Lockhart-Martinelli is used for dispersed flow with modifications for bubble, slug, stratified, plug and annular flow regimes. The method of Schneider, White and Huntington (Reference 14) is used in the wave flow regime.

**MOD**ified Panhandle

A modified version of the Panhandle equation for friction pressure drop in gas lines as given by the GPSA (Reference 9). This is widely used for large diameter, long lines in transmission and gas delivery. It includes the effect of gas compressibility and is recommended for fully turbulent flow. Pipeline EFFiciency should normally be specified for this equation. See *Line: Typical Pipeline Efficiency Values Table*

**MUK**herjee Brill

Mukherjee-Brill is used for two phase flow in horizontal, inclined, or vertical pipes. (Reference 23).

**OLI**emans

Oliemans is used for two phase flow in horizontal pipes. (Reference 26)

**ORK**iszewski

Default equation for calculating pressure drop due to friction in two-phase, vertical lines. This method is an extension of earlier work by Griffith and Wallis primarily for slug flow and is a composite of the following methods; 1) Griffith (Reference 11) for bubble flow, 2) Orkiszewski for slug flow friction gradient and 3) Duns and Ros (Reference 13) for transition and

## Chapter 20

---

annular-mist flow, and flow regime determination. The author claims approximately 10 percent precision in predicting pressure drops in flowing and gas-lift production wells.

### **PANhandle A**

Equation for frictional pressure drop in gas lines, mainly applicable to large diameter (6 to 24 inch), long transmission lines. It is an empirical equation appropriate mainly for partially turbulent flow with Reynolds numbers in the range 5E6 to 14E6. The original equation assumes an average temperature of 60F and a gas gravity of 0.6. This calculation has been generalized to use actual flowing temperature and calculated gas gravity. Gas compressibility factor (Z) is not used in this equation. Pipeline Efficiency should normally be specified for this equation.

### **WEYmouth**

Equation for frictional pressure drop in gas lines developed by Weymouth (Reference 7). This version is as modified by GPSA (Reference 9) to include the effects of compressibility factor (Z) and gas gravity. The equation is suitable for fully turbulent flow in short pipelines and gathering systems and gives somewhat conservative results.

---

## **Size Line: Friction Factor Calculation Method**

---

This option is normally set automatically by the METHOD for FRIction. If a friction factor option corresponding to the METHOD for FRIction exists then it is normally used. Otherwise the default friction factor used is MOODY. For comparative purposes Design II allows you to specify friction factor methods independently of the equation for friction pressure drop. Results so obtained should be interpreted with caution since empirical friction factors are only valid for a limited range of conditions. Numerical values of all friction factors reported in the output are always 4 times the equivalent "Fanning friction factor" which is sometimes used, so comparisons with friction factors from other sources should be made with care. The available options are:

### **METHOD for friction FACTor =**

Enter one of the options for calculation of the friction factor for each of the lines on the USE streams command. The default depends on the friction method if specified, otherwise the default is MOODY.

### **AGA**

Friction factor corresponding to the American Gas Association friction pressure drop method. Different equations are used for partially and for fully turbulent flow, reflecting the more sudden transition than that modeled by the Colebrook equation. Drag factor is used to calculate the transition Reynolds number and the friction factor in the partially turbulent flow regime. This is for gas and wet gas lines and is automatically selected if MET FRI = AGA is used. The roughness used to calculate the AGA friction factor is the effective roughness instead of the absolute roughness so a somewhat more conservative value should be used.

### **BEGgs and Brill**

The Beggs and Brill correlation is an integrated method for pressure drop calculation for two phase systems. With specification of BEGgs as the friction pressure drop method all other calculation methods for elevation effects, friction factor, flow regime, and holdup default to the Beggs and Brill technique automatically. (Reference 18)

### **DUKler**

The DUKler correlations for two-phase pressure drop use the constant slip (Case II) method. (Reference 17) Unless you specify otherwise, the DUKler method for friction factor will also be used.

### **JAIN**

Explicit friction factor comparable to the Colebrook equation in the Reynolds number range of 5000 to 108 with relative roughness between 10<sup>-6</sup> and 10<sup>-2</sup>. (Reference 16).

### **MOODY**

General default friction factor corresponding to the widely used Moody chart (Figure 2.) and calculated iteratively from the Colebrook equation. The Moody friction factor represents a smooth and gradual transition into turbulent flow. It can be used for both single and two-phase flow. (Reference 15).

### **PANhandle A**

Friction factor corresponding to the Panhandle A equation for friction pressure drop. This is used automatically if MET FRI = PAN is entered. It predicts lower values than either MOODY or WEYmouth in the valid range of the Panhandle A equation.

### **WEYmouth**

Friction factor corresponding to the Weymouth equation for friction pressure drop. This is used automatically if MET FRI = WEY is entered. It is an empirical correlation of limited validity and was based on air in small diameter pipes. It is not recommended for use in equations other than Weymouth's. It will predict higher friction factors than MOODY for line diameters under 20 inches, and lower friction factors for diameters over 20 inches.

---

## **Size Lines: Elevation Change Pressure Drop Calculation Method**

---

### **METHOD for ELEvation pressure drop =**

Enter one of the options for calculation of the pressure drop due to elevation. One value should be entered for each line in the USE streams command. The default is PHASE density.

### **PHASE density**

This is the default for both single and two-phase flow. In the case of two-phase flow, an average phase density is used

based on the liquid holdup volume fraction. For single-phase flow the liquid or gas density is used. This is the method recommended for all process plant line sizing and for most other situations.

**FLAnigan**

This is intended for long transmission lines in hilly terrain and ignores any pressure gain in downhill sections. It is intended for two-phase gathering systems (Reference 6). The correlation was empirically derived using data from 4 - 10 inch diameter pipe with gas velocities up to 12 ft/sec and liquid to gas ratios of 20 - 1200 bbl/mmscf. Outside the range of this data its validity is doubtful.

**AGA**

For gas transmission lines using the AGA method for friction pressure drop. This incorporates elevation effects into the AGA equation. The MET FRI = AGA command must also be used.

**ORKiszewski**

For vertical upwards flow in the slug flow regime. Orkiszewski (Reference 4) uses the average density term of Griffith and Wallis (Reference 12), which predicts rather higher densities and consequently elevation pressure drop than the PHase density method.

**Size Lines Command Summary**

**Required**

**SIZE LINES**  
**USE** streams =

**Sizing Criteria**

**MAX**imum **DEL**ta P per hundred feet (P units) =  
 (L units/t units) =  
**NOM**inal **DI**Ameter (L units) =  
**MAX**imum **SON**ic fraction =

**Pipe Geometry Specification**

**INS**ide **DI**Ameter (L units) =  
**PI**Pe **WAL**I code =  
**LEN**gth of pipe (L units) =  
**EQU**ivalent length (L units) =  
**DIR**ection of flow =  
**ELE**vation of pipe (L units) =

**Pipeline Transport Efficiency**

**ROU**ghness (L units) =  
**DRA**g factor =  
 pipeline **EFF**iciency = (fraction)

**Pipeline Phase Specification**

**SET** phase of calculation =

**Pressure Drop Calculation Method**

**METH**od for **FR**iction pressure drop =  
**LOCK**hart-Martinelli  
**ORK**iszewski  
**AGA**  
**WEY**mouth  
**PAN**handle A  
**MOD**ified Panhandle

**Friction Factor Calculation Method**

**METH**od for friction **FA**CTOR =  
**DAR**cy-Weisbach  
**MOO**dy  
**JAI**n  
**AGA**  
**WEY**mouth  
**PAN**handle A

**Elevation Change Pressure Drop Calculation Method**

**METH**od for **ELE**vation pressure drop =  
**PH**ase density  
**FL**Anigan  
**AGA**  
**ORK**iszewski

**Size Lines Step by Step**

**Size Lines STEP 1**

*Specify the stream numbers of the lines which are to be sized*

Enter command keyword  
 Enter the stream numbers of the lines which are to be sized

**SIZ LIN**  
**USE =**

**Size Lines STEP 2**

*Choose the line sizing criteria (enter ONE of the following)*

**NOTE:** Only one sizing criteria is allowed per **SIZ**e **LIN**e section. However, multiple **SIZ**e **LIN**e sections are allowed per run to see the effect of different sizing specifications on the same line.

Maximum allowable pressure drops for each of the streams on the **USE** streams command (default is 0.5 PSI per hundred feet)  
 Maximum allowable velocities for each of the streams on the **USE** streams command (units should be specified since the default units are FT/HR *not* FT/SEC)  
 Nominal diameters of each of the lines to be calculated  
 Maximum allowable fraction of sonic velocity for each of the lines on the use streams command

**MAX DEL** (P units) =  
**MAX VEL** (L units/t units) =  
**NOM DIA** (L units) =  
**MAX SON** = (fraction)

**Size Lines STEP 3**

## Chapter 20

### Pipe inside diameter specification. Choose any of the optional line sizing specifications listed below:

Inside diameters of each of the lines on the USE streams command (default is determined from the nominal diameter and the pipe table)	<b>INS DIA</b> (L units) =
Pipe wall thickness specification (select ONE of the following)	
Standard wall	<b>PIP WAL = STD</b>
Extra strong wall	<b>PIP WAL = XS</b>
Double extra strong wall	<b>PIP WAL = XXS</b>
Pipeline length specification (select ANY of the following options)	
Length of the pipe for each line on the USE streams command (Default value is 100 feet)	<b>LEN</b> (L units) =
Equivalent length of bends and fittings for each line on the USE streams command (values will be added to the actual length for calculations; default is zero)	<b>EQU</b> (L units) =
Line flow direction specification (select ONLY ONE of the following three options)	
Horizontal flow (includes inclined horizontal flow)	<b>DIR = HORI</b>
Vertical upwards flow (includes inclined upwards flow)	<b>DIR = UP</b>
Vertical downwards flow (includes inclined downwards flow)	<b>DIR = DOWN</b>
Pipeline elevation changes specifications	
Elevation of the pipe for each of the lines on the USE streams command (positive for upwards inclined flow and negative for downwards inclined flow; default is zero for HORIZONTAL pipe, length of pipe for Upwards flow and negative pipe length for DOWNwards flow)	<b>ELE</b> (L units) =
ABSOLUTE pipe roughness factor specification	
Absolute pipe wall roughness for each of the lines on the USE streams command (default is 0.00015 feet)	<b>ROU</b> (L units) =
Drag factor for the AGA pressure drop equation specification	
Drag factor for use in the AGA equation (should be entered whenever MET FRI = AGA; one value for each line specified in the USE streams command; default is 1.0)	<b>DRA</b> =
Pipeline efficiency factor specification	
Fractional pipeline efficiency for use in the Panhandle A, Modified Panhandle and Weymouth equations (default is 1)	<b>EFF</b> = (fraction)
Line phase specification (select ONE of the following)	
Liquid (default is the phase as determined by the program)	<b>SET = LIQ</b>
Vapor (default is the phase as determined by the program)	<b>SET = VAP</b>

### Size Lines STEP 4

Frictional pressure drop calculation method. Choose any of the optional pipeline sizing calculation methods.	
Darcy-Weisbach (default for gas and liquid)	<b>MET FRI = DAR</b>
Lockhart-Martinelli (default for two phase horizontal)	<b>MET FRI = LOC</b>
Orkiszewski (default for two phase vertical)	<b>MET FRI = ORK</b>
AGA (American Gas Association) for gas (including wet gas)	<b>MET FRI - AGA</b>
Weymouth for gas (including wet gas)	<b>MET FRI - WEY</b>
Panhandle A for gas (including wet gas)	<b>MET FRI = PAN</b>
Modified Panhandle for gas (including wet gas)	<b>MET FRI = MOD</b>
Friction factor calculation method (select ONE of the following)	
Moody (default for single and two-phase flow)	<b>MET FAC = MOO</b>
Jain	<b>MET FAC = JAI</b>
AGA (default if MET FRI = AGA)	<b>MET FAC = AGA</b>
Weymouth (default if MET FRI = WEY)	<b>MET FAC = WEY</b>
Panhandle A (default if MET FRI = PAN)	<b>MET FAC - PAN</b>
Elevation change pressure drop calculation (select ONE of the following)	
Phase density (default for both single and two-phase flow in both vertical and horizontal directions)	<b>MET ELE = PHA</b>
Flanigan	<b>MET ELE = FLA</b>
AGA (default if MET FRI = AGA)	<b>MET ELE = AGA</b>
Orkiszewski	<b>MET ELE = ORK</b>

### Size Lines Examples

There are several sample flowsheets in "Chapter 52: Process Line Sizing Samples - c:\designiisamples\size\_line" of the DESIGN II for Windows Tutorial and Samples Guide.



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# Index

Add Inline FORTRAN Statements .....	276	ChemTran: Surface Tension Methods.....	241
Add Optional FORTRAN Commands.....	276	ChemTran: UNIFAC Estimation Technique for Activity	
Calculation Options Step 1 .....	136	Coefficients.....	244
Calculation Options STEP 2 .....	136	ChemTran: Unified Group Contribution Technique .....	242
Calculation Options STEP 3 .....	137	ChemTran: Using ChemTran to Output Component Physical	
Calculation Options: Calculate Dew/Bubble Points, Heating Values		Properties .....	257
& Wobbe Index .....	137	ChemTran: Using the Modified Peng-Robinson Equation of State	
Calculation Options: Checking For CO <sub>2</sub> Freeze-Up .....	139	.....	257
Calculation Options: Condensate Recovery.....	141	ChemTran: Using the Structure Command to Define a Custom	
Calculation Options: Execution Control .....	131, 135	Component.....	256
Calculation Options: Heating Curve.....	140	ChemTran: Vapor Pressure Methods .....	237
Calculation Options: Hydrate Formation Prediction.....	139	ChemTran: Volume (Density) Methods.....	239
Calculation Options: Lost Work.....	135	ChemTran: When to Use ChemTran.....	180
Calculation Options: Lost Work Analysis .....	141	Component by Component Command Details.....	71
Calculation Options: Standard Conditions.....	134	Component by Component Crude Feed Command Summary .....	74
ChemTran STEP 1.....	249	Component by Component Examples.....	74
ChemTran STEP 2.....	249	Component by Component Optional Commands.....	72
ChemTran STEP 3.....	249	Component by Component Other Property Specifications .....	73
ChemTran STEP 4.....	249	Component Database - ID From 1 to 99 .....	11
ChemTran STEP 5.....	250	Component Database Sorted By ID .....	11
ChemTran STEP 6.....	250	Component Properties Estimation Methods.....	51
ChemTran STEP 7.....	250	Component Properties Stored .....	50
ChemTran: Acentric Factor Methods .....	238	Crude Bulk Feed Command Details.....	61
ChemTran: Application of the Structure Command .....	243	Crude Bulk Feed Command Summary .....	70
ChemTran: Applications.....	179	Crude Bulk Feed Example	
ChemTran: Calculating Binary Interaction Parameters by		Specification Using TBP Distillation Curve .....	69
Regressing VLE Data .....	255	Crude Bulk Feed Optional Properties .....	65
ChemTran: Calculating Binary Interaction Parameters from Infinite		Crude Bulk Feed STEP 1.....	68
Dilution Activity Coefficients.....	256	Crude Bulk Feed STEP 2.....	68
ChemTran: Calculating Binary Interaction Parameters from Infinite		Crude Bulk Feed STEP 3.....	68
Dilution Activity Coefficients Estimated from UNIFAC .....	256	Crude Bulk Feed STEP 4.....	68
ChemTran: Calculating Binary Interaction Parameters from Infinite		Crude Bulk Feed STEP 5.....	68
Dilution Activity Coefficients using Regular Solution Theory.....	256	Crude Bulk Feed STEP 6.....	69
ChemTran: Characteristic Volume Method.....	239	Crude Bulk Feed STEP 7.....	69
ChemTran: Component Properties Command Details.....	215	Crude Bulk Feed STEP 8.....	69
ChemTran: Correlation Equations , Procedures and Parameters		Crude Bulk Feed Step by Step.....	68
ChemTran: Critical Property Methods.....	232	Crude Oil Library Command Details	
ChemTran: Database List .....	179	feed stream initialization	
ChemTran: Electrolyte Command Details.....	186	composition specification	
ChemTran: Electrolyte Component Library .....	185	flowrate specification	
ChemTran: Electrolyte Component Theory.....	185	temperature and pressure specification.....	79
ChemTran: Electrolyte Input File .....	187	Crude Oil Library Command Summary.....	80
ChemTran: Electrolyte System Data .....	186	Crude Oil Library Example.....	80
ChemTran: Entering Data for Pseudo Components (100) and		Crude Oil Library Table.....	79
Chemical Components (200) .....	253	DESIGN II Ionic Component Library.....	51
ChemTran: Entering Data for Solid Components (300) .....	255	Flowsheet Optimization Input Commands.....	259
ChemTran: Entering Experimental or Literature Values for Binary		Flowsheet Optimization: Basic Problem Definition.....	262
.....	255	Flowsheet Optimization: Constraints .....	263
ChemTran: Entering Properties to Define a Custom Component.....	253	Flowsheet Optimization: General Discussion .....	262
ChemTran: Example Input File .....	181	Flowsheet Optimization: Maximum Search Step.....	265
ChemTran: Executing ChemTran.....	180	Flowsheet Optimization: Objective Function.....	263
ChemTran: Global Output Unit Specification .....	181	Flowsheet Optimization: Perturbation Size.....	264
ChemTran: Guidelines for Regressing Equilibria Data .....	251	Flowsheet Optimization: Scaling .....	264
ChemTran: Ideal Gas Heat Capacity Methods.....	233	Flowsheet Optimization: Solution Tolerances .....	264
ChemTran: Input Commands for Single Components .....	212	Flowsheet Optimization: Table 1. Design Variable list for OPTIM	
ChemTran: Introduction to Mixtures .....	188	Section .....	265
ChemTran: Ionic Reaction Library.....	186	Flowsheet Optimization: Table 2. DESIGN II Utilities Available in	
ChemTran: Latent Heat Methods.....	240	OPTIM Section .....	267
ChemTran: Mixture Command Details.....	194	In a FORTRAN Library.....	275
ChemTran: Mixture Data Entry .....	180	In DESIGN II Equipment Module Sections.....	274
ChemTran: Normal Boiling Point Estimation.....	229	In user-defined equipment modules (ADD block).....	275
ChemTran: Phase Equilibrium Data Entry .....	208	Inline Fortran	
ChemTran: Pure Component Optional Commands .....	242	Arithmetic Operators.....	279
ChemTran: Pure Component Physical Property Entry, Regression		DESIGN II Flash Subroutine .....	279
and Estimation .....	179	DESIGN II Utility Subroutines.....	278
ChemTran: Pure Component Required Commands.....	241	Distillation Functions .....	277
ChemTran: Selecting Correlations for Mixture Data.....	200	Equipment Parameters .....	277
ChemTran: Solubility Parameter Method.....	240	Intrinsic Functions .....	279

# Index

Keywords.....	280	Specifying Feed STEP 2 .....	59
Pure Component Physical Property Data .....	278	Specifying Feed STEP 3 .....	59
Relational and Logical Operators .....	280, 281	Specifying Feed STEP 4 .....	60
Stream Properties.....	277	Specifying Feed STEP 5 .....	60
Thermodynamic Interaction Parameter Banks .....	278	Thermodynamics Quick Guide .....	105
Thermodynamic Library Subroutines 1 .....	278	Thermodynamics STEP 1 .....	102
User Added Equipment Modules ADD Blocks .....	272	Thermodynamics STEP 2 .....	102
Inline Fortran: Activity Coefficient Equations Binary Interaction Parameter.....	291	Thermodynamics STEP 3 .....	103
Inline Fortran: Existing Equipment Module Modifications .....	269	Thermodynamics STEP 4 .....	104
Inline Fortran: General Parameters .....	277	Thermodynamics STEP 5 .....	104
Inline Fortran: Review FORTRAN Coding .....	276	Thermodynamics STEP 6 .....	104
Inline Fortran: Subroutines for both Existing Equipment Modifications and ADD Blocks.....	273	Thermodynamics STEP 7 .....	105
Input Units STEP 1 .....	164	Thermodynamics Table 1. APISOAVEK Interaction Parameter List .....	107
Input Units STEP 2 .....	164	Thermodynamics Table 3. Peng Robinson Binary Interaction Parameters.....	84, 108, 114
Input Units: Default Temperature and Pressure Units .....	166	Thermodynamics Table 4. Lee- Kesler Binary Interaction Parameters.....	83, 89, 93
Input Units: Discharge Pressure Units .....	166	Thermodynamics Table 5. Henry's Constants in Water List . 87, 88, 119	
Input Units: Temperature and Pressure Units .....	166	Thermodynamics Table 6. Mixed Amine Modeling ...	119, 122, 123
Output Units STEP 1 .....	169	Thermodynamics: Critical Properties and Acentric Factor Specification .....	98
Output Units STEP 2 .....	169	Thermodynamics: Data Factors Tc, Pc, MW Calculation Options	99
Output Units: Global.....	169	Thermodynamics: Enthalpy (H) And Entropy (S) Options .....	88
Output Units: Global SI Units with Time Units.....	170	Thermodynamics: Enthalpy Datum .....	91
Output Units: Liquid and Vapor Outlet Units.....	170	Thermodynamics: Heat of Formation and Entropy of Formation Specification .....	100
Output Units: Quantity .....	169	Thermodynamics: Heating Value Specification.....	100
Petroleum Fraction Optional Commands.....	57	Thermodynamics: K-Value Commands .....	82
Print Options STEP 1 .....	146	Thermodynamics: Mixed Amine Models.....	97
Print Options STEP 2 .....	146	Thermodynamics: Mixed Amine Notes .....	97
Print Options: ASTM 86 Distillation.....	147	Thermodynamics: Mixed Amine Physical Properties .....	98
Print Options: Format Control .....	143	Thermodynamics: Peneloux Correction to Soave Density .....	100
Print Options: Ionic Stream Output Control .....	144	Thermodynamics: Relative Speed of K-Values .....	88
Print Options: Petroleum Stream Output Control .....	144	Thermodynamics: Selecting Enthalpy Option.....	91
Print Options: Plot Output Control .....	145	Thermodynamics: Selecting K-Value Options.....	88
Print Options: Standard Output Control.....	143	Thermodynamics: Surface Tension Options .....	96
Print Options: Stream Naming Command .....	144	Thermodynamics: Thermal Conductivity Options .....	95
Print Options: Stream Summary .....	146	Thermodynamics: Viscosity Options .....	94
Print Options: Use of the PLOT commands .....	149	Thermodynamics: Water K-Values in Hydrocarbon Systems.....	81
Real Feeds Command Details.....	53		
Real Feeds Command Summary.....	55		
Recycle Loops STEP 1 .....	156		
Recycle Loops STEP 2 .....	156		
Recycle Loops STEP 3 .....	156		
Recycle Loops: Case Study .....	154		
Recycle Loops: Control .....	154		
Recycle Loops: Direct Substitution .....	152		
Recycle Loops: Example .....	154		
Recycle Loops: Simultaneous Convergence .....	152		
Recycle Loops: Specified Sequence .....	153		
Recycle Loops: Wegstein .....	151		
Size Line References .....	309		
Size Line: Friction Factor Calculation Method.....	306		
Size Lines STEP 1 .....	307		
Size Lines STEP 2 .....	307		
Size Lines STEP 3 .....	308		
Size Lines STEP 4 .....	308		
Size Lines: Elevation Change Pressure Drop Calculation Method .....	306		
Size Lines: Pipe Geometry Specification.....	304		
Size Lines: Pipeline Phase Specification .....	305		
Size Lines: Pipeline Transport Efficiency.....	304		
Size Lines: Pressure Drop Calculation Method .....	305		
Size Lines: Required Commands.....	304		
Size Lines: Sizing Criteria Commands .....	304		
Sizing, Process Line .....	251, 267, 281, 309		
Specifying a Feed Stream step 1.....	58, 59		
step 2.....	58, 59		
Specifying Feed STEP 1 .....	59		