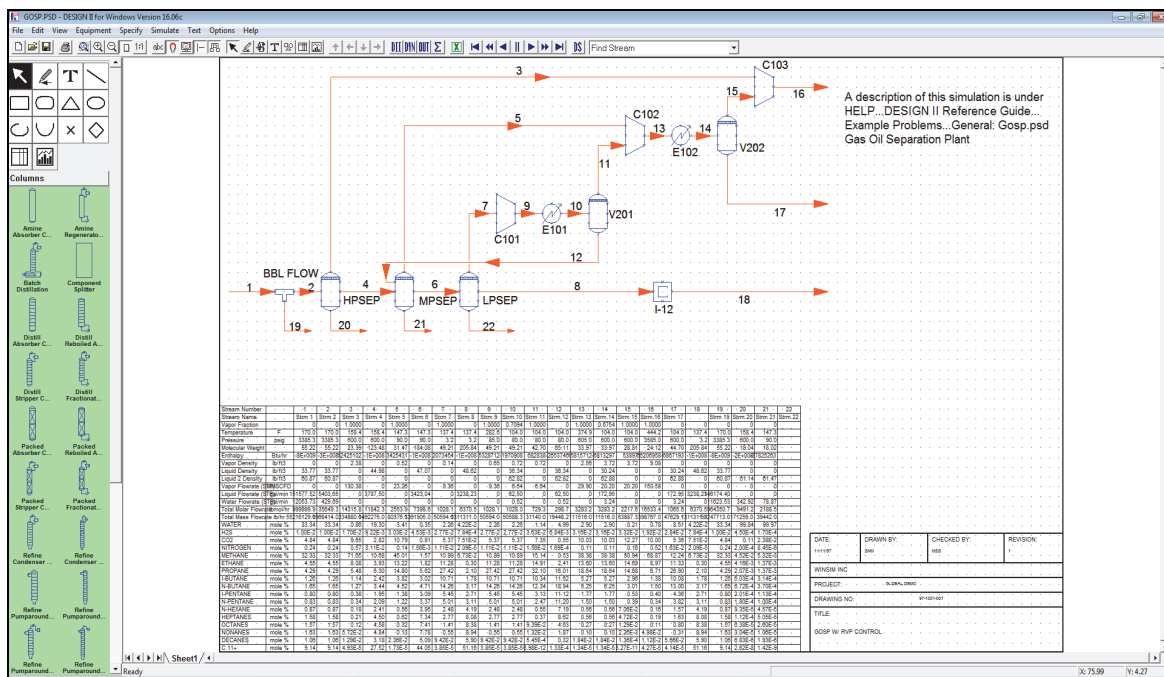


DESIGN IITM

Unit Module Reference Guide Version 16.0



WinSim® Inc.

Advanced Engineering Software

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Chapter 1: Equipment Modules

Equipment Modules: Column Calculations

Amine Column
Batch Distillation

Component Splitter
Distillation Column

Packed Column
Refine Column

Shortcut Fractionator
Stream Manipulator

Equipment Modules: Heat Exchange

Air Cooled Exchanger
Double Pipe Exchanger

Fired Heater
Heat Exchanger

LNG Exchanger
Multiple Flashes

Plate – Fin Exchanger

Equipment Modules: Pressure Change

Compressor
Expander

Expander Compressor Line
Pressure Drop

Multiple Flashes
Polytropic Compressor

Pump
Valve

Equipment Modules: Reactors

Continuous Stirred Tank Reactor
Equilibrium Reactor

Hydrotreater
Plug Flow Reactor

Reactor
Stream Manipulator

Equipment Modules: Sizing

In addition to solving complex flowsheet simulations via rigorous heat and material balance, DESIGN II performs calculations that are useful and time saving to a process design. These features are available during flowsheet simulation. They do not require a separate computer run. These features include:

Air-Cooled Exchanger Rating

The exchanger may be rated for two service types, namely either cooler or air condenser. The two draft types designed are induced and forced draft using axial flow, propeller type fans to drive ambient air at local atmospheric pressure across a rectangular tube bundle. Rating mode determines airflow for fully specified geometry (physical data on fin, fan, and tubes) and process conditions. Airside heat transfer and pressure drops are calculated from a general correlation. See Air-Cooled Exchanger Rating Section.

Depressuring

Calculates pressure buildup in a closed vessel until the pressure reaches the value specified for the set pressure of the relief valve. The conditions during the blowdown period after the depressuring valve opens are shown. The blowdown period is divided into several specified intervals with important variables reported at each interval. See DEPRESsuring Section.

Distillation Tray Sizing

There are two different shortcut sizing techniques in the Distillation column calculations, *Smith-Dresser-Ohlswager Technique* and *Glitsch Technique* (Glitsch Bulletin 4900). Both calculations are performed automatically using default values unless you change one or more available commands. For details, see Distillation: Tray Sizing Section.

Flow Meter Sizing

Flow Meter allows square-edge, quadrant, and conical type orifice plates to calculate the size of the orifice, flow rate of the stream, or the pressure drop across the orifice.

Heat Exchanger Rating

Rigorous rating of liquid, vapor, and two-phase heat exchangers. This feature calculates pressure drop, heat transfer coefficients, and heating or cooling requirements. See Heat Exchanger: Rating Commands Section.

Plate-Fin Exchanger Rating

The rating calculations are performed for plate-fin exchangers. Rating calculation using the geometry (fin, plate and configuration details) specifications you have entered is used to calculate outlet stream temperatures and total duty. See

Chapter 1

Plate-Fin Exchanger: Rating Section.

Process Line Sizing

Single and two-phase lines can be sized to meet your specification of pressure drop, velocity, sonic velocity fraction, or nominal diameter. See Size Line: Required Commands Section.

Separator Sizing

Sizes any single stage separator in the flowsheet. Sizing can be performed on any vertical or horizontal vapor-liquid separation e.g. flash drums, compressor inlet separators, etc. See Valve: Separator Sizing Commands or Flash: Separator Sizing Sections.

Transmission Line

Calculates pressure drops due to friction and elevation change (if any) in transmission lines or plant piping of specified length and diameter. Additionally performs calculations for back pressure, diameter case studies, and liquid holdup. See [LINE](#) Pressure Drop Optional Command Details Section.

Equipment Modules: Stream Operations

Component Splitter
Divider
Flash

Line Pressure Drop
Mass Balance
Mixer

Multiple Flashes
Multiple Phase Flash
Stream Manipulator

Valve

Equipment Modules: Equipment Control

Controller

Equipment Modules: Auxiliary Modules

Add Module
Depressuring

Flow Meter
Phase Envelope

Phase Map

Equipment Modules: Thermodynamic Method Optional Commands

Use these commands to specify options for the module only when they are different than the system **thermodynamic methods** specified in the General commands. Additional keywords for different methods are given in the Thermodynamics Section.

HKEY =

Enter symbolic name for enthalpy option. (e.g. **HKE** = SOAVEH)

KKEY =

Enter symbolic name for K-value option.(e.g. **KKE** = SOAVEK)

DKEY =

Enter symbolic name for density option.(e.g. **DKE** = COPED)

LIQUID DKEY =

Enter symbolic name for density option (e.g. **LIQUID DKEY** = PEND)

VSVKEY =

Enter symbolic name for vapor viscosity option. (e.g. **VSVKEY** = DEAN)

VSLKEY =

Enter symbolic name for liquid viscosity option. (e.g. **VSLKEY** = API)

THVKEY =

Enter symbolic name for vapor thermal conductivity option. (e.g. **THVKEY** = NBS81)

THLKEY =

Enter symbolic name for liquid thermal conductivity option. (e.g. **THLKEY** = TEMA)

STKEY =

Enter symbolic name for surface tension option. (e.g. **STKEY** = API)

Water Immiscibility

IMM = 62

Enter if water is to be treated as an immiscible component.

NO IMM

Enter if water is NOT to be treated as an immiscible component (becomes miscible).

NOTE:

1. These options are **NOT** available for the Flowmeter, Batch, and Controller modules.
2. The Mixed Amine thermodynamic method (KKE=AMINEK and HKE=AMINEH) is NOT available for individual equipment modules as an option. This method can only be selected as an overall thermodynamic method of choice.

Chapter 2: Add Module

ADD Blocks are user-written FORTRAN models of equipment that 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. Compilation and linkage steps, which are internal to DESIGN II, are automatic.

The ADD Module feature in DESIGN II allows you to use your own process technology in conjunction with the standard equipment modules. To use the ADD Modules(s), you must write your own FORTRAN subroutine(s) to interface with DESIGN II, which will perform the additional calculations in the course of the simulation. Typical applications for ADD Modules include the following:

Economic Evaluations

Substituting Unit Calculation Techniques

Simulation of Proprietary Unit Operations

Pollution Calculations

Add Module: Command Details

A working knowledge of FORTRAN is necessary for writing ADD module subroutines. In addition, the commands needed to construct the program interfaces are different than the English-language input used throughout DESIGN II. Detailed guidelines for using the ADD modules are presented below:

This describes how users may write ADD BLOCKS (user written subroutines), to perform calculations which are not normally carried out by DESIGN II. It is a useful facility to ADD equipment modules to the DESIGN II program for processes which cannot otherwise be simulated. The following describes such an option and needed coding for subroutines:

For specifics on writing the subroutine, please refer to Chapter 8.4 Inline Fortran.

Add Module: Requirements

- The ADD block module must be designed so that outlet stream conditions are calculated from inlet stream conditions, not vice versa. In other words inlet stream compositions, temperatures, and pressures must be specified, and the outlet stream compositions, temperatures, and pressures calculated by the module.
- The ADD block must be structured as a Fortran subroutine with a single entry point and a single return point, and with the calling sequence specified below. Any parameters required will be input via "equipment parameters" discussed later. It may call other subroutines as part of its calculations. Any such subroutines should transfer data by means of calling arguments rather than COMMON blocks.
- Any results printed in the ADD block should be printed using Fortran logical unit 6. For a new page use the subroutine PTITLE as shown below to preserve correct page numbering sequence. It is CALL PTITLE. You may write to the console using Fortran logical unit 1.
- For every Fortran WRITE instruction, you should first call the subroutine LINECK to adjust the line count correctly. If a new page is required it will be handled automatically. CALL LINECK (N), where N is the number of lines printed.
- Error conditions which may occur during the calculation should be handled in the following way. An error message indicating the subroutine name and the type of error should be printed using Fortran logical unit number 6. If the error occurs in a subroutine of the ADD block, an error flag should be set as one of the parameters in the calling sequence and control returned to the calling subroutine. After every subroutine call, the error flag must be tested. If an error is indicated, control must be returned to the ADD block which in turn must set a "stop indicator" and return control to the DESIGN II program.

Add Module: Inline FORTRAN Add Blocks

This feature allows the user to write Fortran statements directly into any part of the DESIGN II input without the need for separate compilation and linking.

When using the Inline FORTRAN Add Blocks, the subroutine FORTRAN statements are entered directly into the DESIGN II input- together with the normal DESIGN II input commands. Each time the DESIGN II input is submitted for execution the FORTRAN sections are automatically compiled and linked into DESIGN II internally at the beginning of the run. If any compilation or linkage errors occur, the run stops and full descriptive error messages are provided.

Inline FORTRAN can also be used to modify the calculations performed by existing unit modules. For modifying calculations performed by existing unit modules, please see the special features section under Inline Fortran Command Details

Add Module: 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.

Chapter 2

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.

NEQp = 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 *par 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 *Inline Fortran: Table 8. DESIGN II Flash Subroutine (use with CALL)*).
4. Return all output stream information to DESIGN II.

Add Module: Essential Data Interface within ADD Blocks

FORTTRAN statements in ADD blocks can be viewed as independent of DESIGN II. However, in order to transfer data back and forth between DESIGN II and the ADD Block, variable names must be connected to the equivalent variable names in DESIGN II. This connection is done by the conventional FORTRAN method of subroutine arguments. These arguments or variables can be divided into four categories:

Stream Parameters

This consists of Component flowrates, Temperature, Pressure and Properties for inlet streams to the ADD Block, and corresponding calculated quantities for outlet streams.

NCP

(scalar), Number of components.

SIVPFR

(vector, length equal to the number of inlet streams (NIN)) Vapor fractions of inlet streams.

SITEMP

(vector, length NIN) Temperatures of inlet streams in R.

SIPRES

(vector, length NIN) Pressures of inlet streams in PSIA.

SIENTH

(vector, length NIN) Enthalpies of inlet streams in BTU/HR.

SIMOLE

(vector, length NIN) Total lbmol/hr of inlet streams.

SICOMP

(matrix, NCP by NIN) Mole fraction composition for each inlet stream.

SIKV

(matrix, NCP by NIN) K-values of each component for each inlet stream.

SOVPFR through SOKV

are the same as SIVPFR through SIKV except they are for the outlet streams. The number of outlet streams, (NOUT) replaces NIN.

ADD block inlet stream parameters are automatically available in the ADD block subroutines. Outlet stream parameters for all output streams must be set by the ADD block in one of two ways:

1. If there is no change in either material or energy from inlet to outlet, simply copy the inlet stream information into the corresponding outlet stream variables. For example,

$$SOTEMP(1) = SITEMP(1)$$
2. If there is a change in composition (e.g. reaction), temperature or pressure from inlet to outlet, then the FLASH1 subroutine (adiabatic or isothermal) must be performed at the outlet conditions to determine stream K-values, vapor fraction, and enthalpy for the outlet stream(s), (See Table 8).

NOTE: The GET and SET functions should not be used in the block to alter parameters of the ADD block's inlet streams or outlet streams. Any manipulation of these stream parameters must be done by directly accessing the stream parameters as described here. The GET and SET functions may be used from within the ADD block on other flowsheet streams just as in any other equipment module.

Equipment Parameters

These are the input variables specifically required by the ADD Block, together with any calculated quantities which may need to be referenced later in the flowsheet. These are transferred as arguments in the calling sequence by using the EQP input keyword command. These are defined in the input as values in the EQP keyword command. They are available in the ADD block as EQPAR(n), where n is the position in the list.

NEQ is the number of equipment parameters used and must be specified in the input file with the NEQ = k keyword command. Note that the first equipment parameter is reserved for the equipment number (on the flowsheet), so user defined input or output parameters may start with EQPAR(2). Minimum value for NEQ should be 2; one for the equipment number and one for the flash type (adiabatic or isothermal)

- General Equipment Module Parameters
- These are normally necessary for ADD Block calculations and must not be modified by the ADD Block, with the exception of ISTOP.

NIN

Number of inlet streams to the ADD Block, set up automatically.

NOUT

Number outlet streams from the ADD Block, set up automatically.

NCP

Number of components in the process flowsheet, set up automatically.

IDCOMP

Component ID numbers (array is NCP in length) used in the flowsheet. This is set up automatically in the order they are entered on the COMponent command in the GENeral section.

KTRACE

Key for trace output which can be useful to obtain diagnostics while testing your ADD Block. Use values of KTRACE greater than 99000.

ISTOP

Stop indicator. This is used to trap fatal errors occurring in your ADD Block or one of its subroutines. When such an error occurs, print an error message. To return control to the ADD Block, set

$$ISTOP = EQPAR(1) + 0.5$$

and execute a RETURN from the ADD Block. If no such error trap is used, the program will simply continue execution through as many equipment modules, including recycles, as there are in the flowsheet.

- Physical Properties Parameters
- The component properties available to the ADD Block are molecular weights and normal boiling points. They are available as vectors AMW and ATB in the ADD block. Entries in these vectors have a one-to-one correspondence to the components listed in the GENeral section COMponents command and in the IDCOMP vector.

AMW

(vector, length NCP), Molecular weight of each component

ATB

(vector, length NCP), Normal boiling point in R for each component

Typical Add Block Structure

The following example shows a skeleton structure of a DESIGN II input file which includes an ADD block module consisting of two subroutines, A and B

```
DUMMY OUTLINE OF ADD BLOCK USAGE
HEA EXC 10 = . . .
FLA 2 = . . .
PUMP5 = . . .
```

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```
ADD 1 = MODA, 3, 4, -5,
USE BLOCK 1
NEQ = 5,
EQPAR = 1, 0, .98, .02, 0
F-      PRE
F-      SET(ADD(1),EQPAR(2)) = GET (HEA EXC(10), DUT)
HEA EXC 11 = . . .
F-      SET(HEA EXC(11), DEL TEM) = GET (ADD(1), EQPAR(5))
FORTTRAN
BLOCK 1 = 2, A, B
START LIBRARY
      SUBROUTINE A ( NIN,      NOUT,      NCP,      NEQP,      NDSP
& SIVPFR, SITEMP, SIPRES, SIENTH, SIMOLE, SICOMP, SIKV,
& SOVPFR, SOTEMP, SOPRES, SOENTH, SOMOLE, SOCOMP,
& SOKV,  EQPAR,  DESPAR, AMW,      ATB,      IDCOMP,
& ISTOP, KTRACE)
      EQPAR(5) = EQPAR(3) * EQPAR(4)
      .
      CALL B (argument list)
      .
      RETURN
      END
      SUBROUTINE B (argument list)
      .
      .
      .
      RETURN
      END
STOP LIBRARY
END
```

The ADD 1 module calculation is called after completing the PUMP 5 module calculations. The ADD 1 module name is MODA. There are two inlet streams to the module (3 and 4) and one outlet stream (5). Any stream information or physical properties of the two inlet streams can be accessed in ADD 1 subroutines. There are 5 equipment parameters allocated for ADD 1 calculations. EQPAR(1) must always be the flowsheet equipment number (1, in this case).

EQPAR (3) and EQPAR(4) are values entered by the user (0.98 and 0.02) that will be used in the subroutine calculations. By entering zeroes in EQP positions 2 and 5, space has been allocated for values accessed from other parts of the program. EQPAR (2) has been filled with the duty for HEA EXC 10 by using the Inline FORTRAN GET function. EQPAR(5) will be filled with a value calculated within the ADD 1 subroutine A.

The ADD 1 module calls BLOCK 1, which consists of two subroutines, A and B. Subroutine A is automatically called first since it is listed first in the BLOCK command. It acts as the main, or driver, program for ADD 1. After performing initial calculations, subroutine B is called by subroutine A. When subroutine B calculations are completed, subroutine A calculations are then completed and the ADD 1 block is completed. Sequencing then proceeds to the HEA EXC 11 module. Note that ADD 1, EQPAR(5) can now be accessed by HEA EXC 11 and input as the temperature rise.

Add Module: Placement of Subroutines Within ADD Blocks

Various ADD module subroutines (i.e., a set of FORTRAN calculations that can be performed repeatedly within a program) is to be placed within a separate section. This is accomplished in DESIGN II by adding a new input section which begins with the keyword command, **FORTTRAN**.

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:

F- 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.

F- 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
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.

Add Module: Design II Coding for an Add Module

The DESIGN II coding for an ADD module using Inline FORTRAN is shown below. Please note that additional statements are required when using Inline FORTRAN to indicate the section of the DESIGN II input that is to be read as FORTRAN statements.

Add Block Inline Fortran Coding

An example for Inline FORTRAN would be:

```
ADD8=TEST, 10,-20,-30,
USE BLOCK 3,
NEQP=21
EQP= 8, 10, 40, 3, 14, 21, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
and in the GENERAL section there would be :
FORTRAN
BLOCK 3=1, MAIN
START LIBRARY
SUBROUTINE MAIN ( argument list )
. . .
. . .
RETURN
END
STOP LIBRARY
```

Where:

ADD8=TEST, 10, -20, -30 indicates an ADD module, having flowsheet equipment number 8, name TEST, with one stream in (Stream 10) and two streams out (Streams 20 and 30).

USE BLOCK 3 tells the program which block of FORTRAN code to use for this ADD module.

NEQP=21 is the number of equipment parameters required by the ADD BLOCK.

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EQP= . . . is data for the equipment parameters. The first parameter value after the = sign (ie EQP=8, . . .) is the equipment number of the ADD module on the flowsheet (8 in this example).

BLOCK 3=1, MAIN indicate how many subroutines are in BLOCK 3, (eg in this example there is 1) and the subroutine names, ie MAIN.

START LIBRARY and STOP LIBRARY tell DESIGN II to read statements between START and STOP as FORTRAN statements.

Add Block: Subroutine Data Transfer

Most of the data needed by the ADD BLOCK is exchanged with DESIGN II by the subroutine arguments. Results calculated by the ADD BLOCK are returned to DESIGN II by other subroutine arguments.

Add Block: Stream Information

For both the inlet and outlet streams of the ADD module this consists of :

- Component flowrates
- Temperatures
- Pressures
- Properties (ie K-values, vapor fractions, and enthalpies)

The values for the inlet streams are set up automatically by DESIGN II. If there is no change in stream conditions (material or energy) in the ADD BLOCK, then the inlet stream information is copied into the outlet stream variables. However, if there is some change in the stream conditions (eg adiabatic pressure drop, reaction), then an isothermal flash must be performed at the outlet conditions in order to determine the outlet stream properties (i.e. K-values, vapor fractions, and enthalpies). Such stream actions must be performed by the subroutine and must be included by the user in the ADD BLOCK coding.

Add Block: Equipment Command Parameters

These are the user-provided input specifications required by the ADD subroutine for its calculations in addition to the stream information. This data is input by the user with the EQP= command in the DESIGN II ADD module input.

The number of equipment parameters used must be specified in the input data. Note that the first equipment parameter is reserved for the equipment number (on the flowsheet), so user defined input or output parameters must start with parameter 2. Equipment parameters are transferred as arguments in the calling sequence.

There is also the flexibility to have equipment parameters (which have been calculated by the subroutine) accessible by other equipment in the flowsheet.

Add Block: Flowsheet Control Variables

These variables are normally necessary for your ADD block calculations and must not be modified by the ADD block, with the exception of ISTOP.

- NIN - the number of inlet streams to the ADD module (set up automatically)
- NOUT - the number of outlet streams from the ADD module (set up automatically)
- NCP - the number of components in the flowsheet (set up automatically)
- IDCOMP - the ID numbers of the components
- KTRACE - key for trace output which can be useful to obtain diagnostics while testing your ADD block
- ISTOP - Stop indicator. This is used to trap fatal errors occurring in your ADD block or one of its subroutines. When such an error occurs, print an error message, return control to the ADD block, set...ISTOP =EQPAR(1) + 0.5 and execute a RETURN from the ADD block. If no such error trap is used, the program will simply continue execution through as many equipments, including possibly recycles, as you have in your flowsheet.

The KTRACE and ISTOP variables are used for diagnostics and error trapping respectively. There are usually set within the subroutine to certain allowed values. The remaining variables are determined by the DESIGN II input code and set automatically by DESIGN II. These must not be changed within the subroutine.

Add Block: Physical Properties

Certain physical properties, namely component molecular weights and boiling points, are available directly from the subroutine argument list. All component will be in the same order as given in the COMPONENTS= command in the GENERAL section of the DESIGN II input.

For example, you may wish to print the boiling point of Ethane (component ID = 3), which is present in the COMPONENTS = command, from your ADD BLOCK. Then the following FORTRAN statements will find and print the normal boiling point in whatever position ethane appears in the COMPONENTS = command

```
...  
J=0  
DO 10 I=1, NOCOMP  
IF ( IDCOMP ( I ) . EQ. 3 ) J=I  
10 CONTINUE  
PRINT AMW (J)  
WRITE ( 6,100 ) ATB ( J ),  
100 FORMAT ( ' The boiling point of Ethane = ' , F13.6, R )  
...
```

where:

IDCOMP are the component ID numbers in the COMPONENTS = command.

NOCOMP is the number of components in the COMPONENTS = command.

ATB (J) is the normal boiling point, R

AMW is the average molecular weight.

Add Block: Subroutine Argument List

The SUBROUTINE statement for ADD BLOCKS is as follows:

SUBROUTINE subroutine name (NIN, NOUT, NOCOMP, NEQP, NDSP,
 * SIVPFR, SITEMP, SIPRES, SIENTH, SIMOLE, SICOMP, SIKV,
 * SOVPFR, SOTEMP, SOPRES, SOENTH, SOMOLE, SOCOMP,
 * SOKV, EQPAR, DESPAR, AMW, ATB, IDCOMP, ISTOP, KTRACE, NCP)

where

NIN is number of inlet streams to the ADD module
 NOUT is number of outlet streams from the ADD module
 NOCOMP is number of components (as is NCP)
 NEQP is number of equipment parameters (maximum 25 in NEQP)
 NDSP is for a second set of equipment parameters if there are more than 25, up to a total of 50 (maximum 25 in NDSP)
 SIVPFR are vapor fractions of inlet streams to the ADD module
 SITEMP are temperatures of inlet streams to the ADD module (R)
 SIPRES are pressures of inlet streams to the ADD module (PSIA)
 SIENTH are enthalpies of inlet streams to the ADD module (BTU/HR)
 SIMOLE are total flow rates of inlet streams to the ADD module (LBMOL/HR)
 SICOMP are component flowrates for inlet streams to the ADD module (LBMOL/HR)
 SIKV are component K-values for inlet streams to the ADD module
 SOVPFR are vapor fractions of outlet streams to the ADD module
 SOKV are component K-values for outlet streams to the ADD module
 EQPAR are equipment parameters (EQP'S)
 DESPAR are second set of equipment parameters (NDSP's)
 AMW are component molecular weights
 ATB are component normal boiling points (R)
 IDCOMP are component ID numbers

ISTOP and KTRACE were explained in Add Block: Flowsheet Control Variables

These variables are dimensional as follows:

DIMENSION SIVPFR (NIN) , SITEMP (NIN) , SIPRES (NIN) ,
 * SIENTH (NIN) , SIMOLE (NIN) , SICOMP (NOCOMP , NIN) ,
 * SIKV (NOCOMP , NIN)

DIMENSION SOVPFR (NOUT) , SOTEMP (NOUT) ,
 * SOPRES (NOUT) , SOENTH (NOUT) , SOMOLE (NOUT) ,
 * SOCOMP (NOCOMP , NOUT) , SOKV (NOCOMP , NOUT)

DIMENSION EQPAR (NEQP) , DESPAR (NDSP) ,
 * AMW (NOCOMP) , ATB (NOCOMP) , IDCOMP (NOCOMP)

Add Block: Dimension Units used within Add Blocks

Within DESIGN II the following units are used for calculations:

Pressure	PSIA
Temperature	Rankine (R)
Flowrate	LBMOL/HR
Enthalpy	BTU/LBMOL
Entropy	BTU/LBMOL/R
Density	LBMOL/FT3
Thermal conductivity	BTU/HR/FT/ F
Viscosity	centipoise (cP)
Surface tension	dynes/cm
Liquid fraction	molar
Vapor fraction	molar
Time	hours (hr)

Data (other than that entered by the user in the EQP LIST) is automatically available in the above units. It is recommended that user- written ADD BLOCKS use the same dimensional units. Therefore when using entered EQP data in standard DESIGN II subroutines the EQP data must be converted to the appropriate units for correct calculation of the ADD module.

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Standard routines are available for the units conversion of the data in EQPAR, but as yet such routines are not available for the conversion of calculated results to the user-input units. These will be available in a later version of DESIGN II. Since it is likely that the user will require input and output units to be the same it may be easier to convert input units directly rather than use the conversion routines.

If users wish to vary the dimensional units they use for the data given in EQPAR, we suggest that you use a "flag" (ie an EQP parameter value) to indicate to the subroutine which dimensional units being entered. So one value of the chosen EQPAR would set the ADD BLOCK for use of metric units, another value for SI and so on.

Add Block: Guidance on Writing the Subroutine

Some general principles can be given that can be applied in order to ensure that the ADD BLOCK is easy to follow for maintenance purposes of if additional features are required at a later date.

1. DOCUMENTATION - Documentation (such as comment statements) within and external to the ADD BLOCK are obvious necessities, and we recommend that 20- 30 percent of the total code is comments and documentation.
2. ITERATION TOLERANCES - If an ADD BLOCK calculates a result by iteration, it is useful to have EQPAR (2) as the convergence tolerance (in percent), and to automatically set a default (usually 0.01) if no value is input.
3. ERROR CHECKING -The first part of the ADD BLOCK should check the data given in EQPAR for errors. The program run must be aborted if errors such as negative pressure or temperatures below absolute zero occur. This avoids wasting computer time or worse when an impossible calculation is attempted.
4. TRANSFERRING CONTROL - Control should be transferred to the final section of the ADD BLOCK when any errors are detected. This section should then deal with the error as follows:
 - an appropriate error message should be written
 - the DESIGN II run is stopped

The DESIGN II run is stopped by setting the variable ISTOP immediately before returning to DESIGN II as follows:

```
ISTOP=EQPAR ( 1 )+0.5
```

5. STOP - Do NOT use the STOP statement.
6. PAGE THROW - Before any data is written out from the ADD BLOCK it is neater to use the utility routine PTITLE, thus starting a new page of output.
7. PUTTING RESULTS IN A FILE Some users may wish the output from the ADD module to be in a file separate to the normal DESIGN II output, for instance when these results are to be used by another program. The manner in which this can be achieved varies from machine to machine and is easier to accommodate on some machines (eg CDC) than others (eg PRIME).
8. HANDLING FREE WATER - One factor of major importance when writing the ADD BLOCK is the possibility of the existence of free water in the streams used by the ADD module for its calculations. If a flash operation is performed with only 1 or 2 outlet streams the only available data concerning free water is its flow rate in variable DECANT. If it is required to perform calculations on the free water phase, then FLASH1 must be coded with 3 outlet streams. Saturated hydrocarbon vapor is automatically placed in the first outlet stream, hydrocarbon liquid (plus dissolved water) in the second, and free water (plus dissolved hydrocarbon gases and dissolved hydrocarbons) in the third.

NOTE: The following must be included when 3 outlets from a flash are used, in case no free water occurs. The ADD BLOCK must set the free water stream variables to zero prior to each flash, by:

```
FLOWO ( 3 )=0.0
```

where

FLOWO (3) is the flow rate of the third outlet stream

Add Block: Specifying Thermodynamics for Add Modules

In common with all other equipment modules, calculations of K-values, entropies, and densities within the ADD module will normally be based on the options (if any) specified in the GENeral section of the DESIGN II INPUT. Also if a change of thermodynamic options is required in the ADD module, these can be input by the use of the KKE=, HKE=, and DKE= subcommands.

For example:

```
ADD1=...  
KKE= APISOAVEK , HKE=APISOAVEH, DKE=STDD
```

Add Block: Purpose of the Add Module

The object of the ADD module is to calculate seven fluid properties of the stream at various temperatures and pressures and arrange these in a table (file). The properties can then be accessed by another program.

The properties calculated are:

1. Vapor densities (in kg/m³)
2. Liquid densities (in kg/m³)
3. Vapor Viscosities (in centipoise)
4. Liquid Viscosities (in centipoise)
5. Surface tension (in dynes/cm)

6. Mass fraction Vapor
7. Enthalpy of mixture (in kcal/kg)

Input data in the EQP= list specifies the temperatures and pressure, at which the properties are calculated. Each property is calculated at each of the temperature and pressure determined by the EQP= list. In the example there are 3 temperatures (50, 72.5 and 95C) and 3 pressures (1 , 115.5 , 230 BAR), so each property is calculated 9 times.

The results calculated by the ADD module are written as a fixed format data table. See Add Block Example Coding.

Add Block: Module Equipment Parameters

There are seven equipment parameters for the ADD module. They are:

- EQP (1) = equipment number on flowsheet
- EQP (2) = minimum temperature for calculations (C)
- EQP (3) = maximum temperature for calculations (C)
- EQP (4) = number of temperatures to at which to calculate
- EQP (5) = minimum pressure for calculations (BAR)
- EQP (6) = maximum pressure for calculations (BAR)
- EQP (7) = number of pressures at which to calculate

Add Block: Structure of Add Module Subroutine

The subroutine is structured as follows:

Step 1. Dimensional units of input parameters and required units for some of the calculated results are not standard DESIGN II units. Conversion factors are set up:

pressure	density	enthalpy	temperature
----------	---------	----------	-------------

Step 2. Test input parameters for valid input:

- a) number of temperatures (range from 1 to 10)
- b) number of pressures (range from 3 to 10)
- c) minimum temperature (not below absolute zero)
- d) maximum temperature (not less than minimum temperature)
- e) minimum and maximum temperatures only equal if number of temperature is equal to 1
- f) minimum pressure (not negative)
- g) maximum pressure (greater than minimum pressure)

Step 3. Set up variables needed for calculations:

- a) temperatures and pressures used
- b) ADD module inlet stream mass flow

Step 4. Set up variables for call to FLASH1, which is used to calculate stream properties at the temperatures and pressure required. Variables are :

- a) set code for isothermal flash to (EQPAR (2)=1.0)
- b) set number of inlet streams to flash to 1 (NINX =1)
- c) set number of outlet streams from flash to 3 (NOUTX =3) so that liquid property calculation can also be calculated to accommodate free water

Step 5. Perform flash and calculate the 7 properties at desired temperatures and pressures. Calculations are performed within nested loops, where necessary variables being set to zero prior to each call to FLASH1.

Step 6. Write results. The following sequence being repeated for each property:

first line	- number of temperatures and number of pressures
second line	- pressures
third line	- temperatures
fourth line	
fifth line	- calculated property data.
sixth line	

Pressure increasing left to right.

Temperature increasing from top to bottom.

The properties are in the following order:

- vapor density
- liquid density
- vapor viscosity
- liquid viscosity
- surface tension
- mass fraction vapor
- enthalpy of mixture

Step 7. Error section. DESIGN II run stopped when error found.

Add Module Examples

There is a sample flowsheet in “Chapter 8: Add Module Samples - c:\designii\samples\equipment\add” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 3: Air-Cooled Exchanger

An Air-Cooled Exchanger (AIRC) is a device for rejecting heat from a fluid directly to ambient air. This is in contrast to rejecting heat to water and then rejecting it to air, as with a shell-and-tube heat exchanger and a wet cooling tower system.

The obvious advantage of an Air-Cooled Exchanger is that it does not require water, which means that plants requiring large cooling capacities need not be located near a supply of cooling water. An Air-Cooled Exchanger may be as small as an automobile radiator or large enough to reject the heat of turbine exhaust steam condensation from a power plant.

Air-Cooled Exchanger Features

General Features:

The exchanger may be designed for two service types namely either air cooler or air condenser. The two draft types available are induced and forced draft using axial flow, propeller type fans to drive ambient air at local atmospheric pressure across a rectangular tube bundle. The hot process fluid is always considered to be inside the tubes.

Tubes may be low finned, high finned or just cylindrical. High finned tubes are usually radial, circular fins which may be tension wrapped, extruded from a bimetallic liner or embedded into the wall of the tube. Tube bundles are rectangular and may consist of one or more tube rows (or layers). A tube bundle is an assembly of tubes, headers, side frames, and tube supports. Usually the tube surface exposed to the passage of air has extended surface in the form of fins to compensate for the low heat transfer rate of air at atmospheric pressure and at a low enough velocity for reasonable fan power consumption. Tube passes may be specified as single pass or multipass. For two pass coolers, an uneven number of rows per pass may be specified. Fans may be specified as one or more per forced or induced draft type. Air-cooled exchanger determines the air flow in cubic foot per minute, outlet pressure and temperature.

Calculation Types

- Basic air-cooled exchanger without rating can be performed for both single and two-stream exchangers. For a single stream exchanger, air flowrate will be calculated (when not specified) and two specifications (one from the air side and one from process side) can be met. For a two-stream exchanger, one specification is met from the air and process side specifications. (please see Air-Cooled Exchanger Command Details & Air Cooled-Exchanger Optional Commands)
- Air-Cooled Exchanger Rating can be done for a single-stream and a two-stream exchanger types. For a single stream exchanger, air or process stream specifications (one) can be met when geometry (physical data on fin, fan, and tubes) and inlet process conditions are fully specified. For a two-stream exchanger, the specified geometry calculates the air and process outlet conditions along with the estimated fan horsepower. Airside heat transfer and pressure drops are calculated from general correlations.

Air-Cooled Exchanger Command Details

Air-Cooled Single Stream Exchanger (rating off)

A single stream exchanger is defined as an exchanger with only the process stream. Air and process side stream specifications will be met, and air flowrate will be calculated when not specified.

A total of **TWO**-specifications will be met as per user specification, provided ONE from each of listed set of specification commands are chosen.

First Process Side Specification:

One specification is required from the list below when rating is not performed.

TEMperature **HOT CHANGE** (T units) =

Enter the estimate or specified change in temperature for the hot side.

TEMperature **OUT HOT** stream (T units) =

Enter the estimate or specified outlet temperature of the hot side (gives up heat).

TEMperature **APPROACH HOT** side (T units) =

Enter temperature approach between air stream inlet and process stream outlet.

DUTy (H units/ t units) =

Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger.

Second Air Side Specification:

One specification is required from the list below when rating is not performed.

TEMPerature OUT AIR stream (T units) =

Enter the estimate or specified outlet temperature of the air (absorbs heat).

TEMPerature AIR CHAnge (T units) =

Enter change in temperature of the air stream between inlet and outlet.

AIR FLOW rate (Q units/ t units) =

Enter this command to specify the air flowrate for the air-cooled exchanger, if utility fluid is used.

Air-Cooled Single Stream Exchanger (rating on)

When rating is required by the user for a single stream air-cooled exchanger (air flow rate is unknown), the following specification options can be used.

One among the following specifications can be met provided all geometry specifications from Air-Cooled Exchanger Rating section are also specified.

FAN POWER per fan (Power units) =

Enter this command to specify the fan power per fan.

TEMPerature HOT CHAnge (T units) =

Enter the estimate or specified change in temperature for the hot side.

TEMPerature OUT HOT stream (T units) =

Enter the estimate or specified outlet temperature of the hot side (gives up heat).

TEMPerature APProach HOT side (T units) =

Enter temperature approach between air stream inlet and process stream outlet.

DUTy (H units/ t units) =

Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger.

TEMPerature OUT AIR stream (T units) =

Enter the estimate or specified outlet temperature of the air (absorbs heat).

TEMPerature AIR CHAnge (T units) =

Enter change in temperature of the air stream between inlet and outlet.

AIR FLOW rate (Q units/ t units) =

Enter this command to specify the air flowrate for the air-cooled exchanger, if utility fluid is used.

Air-Cooled Two Stream Exchanger (rating off)

A two stream exchanger is defined as an exchanger with both the process and the air streams specified with temperature, pressure, and flow. One specification from the list below for the air (or) process side stream will be met. The specifications are:

TEMPerature HOT CHAnge (T units) =

Enter the estimate or specified change in temperature for the hot side.

TEMPerature OUT HOT stream (T units) =

Enter the estimate or specified outlet temperature of the hot side (gives up heat).

TEMPerature APProach HOT side (T units) =

Enter temperature approach between air stream inlet and process stream outlet.

DUTy (H units/ t units) =

Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger.

TEMPerature OUT AIR stream (T units) =

Enter the estimate or specified outlet temperature of the air (absorbs heat).

TEMPerature AIR CHAnge (T units) =

Enter change in temperature of the air stream between inlet and outlet.

Air-Cooled Two Stream Exchanger (rating on)

A two stream exchanger is defined as an exchanger with both the process and the air streams specified with temperature, pressure, and flow. When the rating is desired, the specified geometry from the Air-Cooled Exchanger Rating section will decide the air and process outlet stream temperatures, along with the calculations for heat exchanged, pressure drops, and the fan horsepower.

There are no specifications required for an Air-Cooled Two Stream Exchanger with rating.

Air-Cooled Exchanger Optional Command Details

TEMPerature AIR IN (T units) =

Enter the inlet temperature for the air stream. If not entered default ambient temperature will be used. Default of **TEMPerature of AMBIent** is 77F.

PREssure OUT HOT (P units) =

Enter the desired discharge pressure for the hot stream. Defaults to feed inlet pressure or frictional delta pressure if **RATING** is turned on.

PREssure OUT AIR (P units) =

Enter the desired discharge pressure for the air stream. Defaults to feed inlet pressure or frictional delta pressure if **RATING** is turned on.

DELta PREssure HOT (P units) =

Enter the desired change in pressure across the exchanger for the hot side stream.

DELta PREssure AIR (P units) =

Enter the desired change in pressure across the exchanger for the air stream.

Q-T

Enter this command to have duty versus temperature curves plotted for heat exchangers.

The Q-T table and plot are useful tools for evaluating exchanger design. These curves are based on end-point temperature results and counter current flow. Since air coolers have cross flow, the minimum temperature approach will not be accurate and may actually show cross-overs which DO NOT actually exist. In addition, bubble points and dew points are marked when vaporization or condensation occurs for hot streams.

Air-Cooled Exchanger Rating

The rating calculations are performed for air-cooled exchangers. All required properties for the rating calculation, such as viscosities, specific heats, densities, phase composition, and mass flows are automatically calculated for inlet and outlet conditions of both streams.

The exchanger may be rated for two service types namely either cooler or air condenser. The two draft types designed are induced and forced draft using axial flow, propeller type fans to drive ambient air at local atmospheric pressure across a rectangular tube bundle.

Rating mode determines airflow for fully specified geometry (physical data on fin, fan, and tubes) and process conditions. Airside heat transfer and pressure drops are calculated from a general correlation.

Air-Cooled Exchanger Calculation Commands

RATING on

You must enter this command to perform a rating calculation.

TYPE of service = number

This is the type of service performed by the air-cooled exchanger. If the choice is NOT entered flash of phase condition in and out determine which type of air-cooler is chosen. TWO choices are available:

- 1 (default) Cooler, single phase, process side
- 2 Condenser, two phase, process side

DRAFT TYPE of air cooler = number

This is the draft type of air-cooled exchanger. TWO choices are available:

- 1 (default) forced draft coolers.
- 2 for induced draft coolers

U-Method = method

This is the calculation method employed for the calculation of mean temperature difference for each stream. THREE

choices are available:

- 1 uses the average difference between the wall and the fluid temperature. This is normally the most stable method.
- 2 uses an average cube root mean temperature difference between wall and fluid.
- 4 log mean temperature difference between wall and fluid (default).

UFActor =

Enter this command to adjust the Overall Heat Transfer Coefficient. It provides a "de-rating" factor for each stream which will be multiplied with the calculated heat transfer coefficient. The default is 1.

AREa (L2 units) =

Enter this command to specify the total finned surface area of the air-cooled exchanger. If number of tubes is specified, area can be calculated from tube geometry (given or defaulted), then the calculated area overrides the AREa (if given).

NUMber of **PAR**allel bundles =

Enter the number of bundles in parallel. This is the total number of bundles of the air-cooled exchanger. The default is 1.

NUMber of **BUN**dles per **BAY** =

Enter the number of bundles per bay. This is the number of bundles per bay of the air-cooled exchanger. The default is 1.

Note: The number of bays is calculated as the ratio of number of parallel bundles to number of bundles per bay.

Air-Cooled Exchanger Fin Commands

FIN Material = number

Enter the choice of fin material. (default is **ALU**minum). Choices are listed below.

If you cannot find the specific tube material in the [Heat Exchanger: Tube Metallurgy Table](#), enter the number for the material which has an average thermal conductivity closest to the desired material.

- 1 **C**ARbon steel
- 2 **A**D**M**iralty brass
- 3 **S**T**A**inless steel 304
- 4 **A**L**U**minum
- 5 **M**ONel
- 6 **R**ED brass
- 7 **C**OPper
- 8 **C**OPper nickel 90/10
- 9 **C**OPper nickel 70/30
- 10 **N**ICKel
- 11 **T**ITanium
- 12 **A**L**L**oy 825
- 13 **C**ARbon **M**OLy Steel
- 14 **S**T**A**inless steel 214
- 15 **G**L**A**ss
- 16 **P**V**C**

FIN Height (L units) =

Enter this command to specify the height of the air cooler fins. Calculated from the outside diameter of the pipe and fin (Fin height = 1/2 fin outside dia - 1/2 pipe outside dia).

FIN Thickness (L units) =

Enter this command to specify the thickness of air cooler tube fins. The default is 0.016 inches.

FIN SH**A**pe =

Enter the choice of fin shape. Choices are listed below

ST**R**aight (default)
EX**T**ruded
TR**I**angular
EM**B**edded

NUMber of **F**INs **P**ER tube length (1/L units) =

Enter the number of fins per inch of air-cooled exchanger tube length. The default for fins/length is 132 fins per foot (11 fins per inch)

Air-Cooled Exchanger Fan Commands

FAN DIAMeter (L units) =

Enter the diameter (from blade tip to blade tip) of the fan. The default is 7 ft.

FAN HUB DIAMeter (L units) =

Enter the diameter of the fan hub (i.e. the central cylinder to which the fan blades are attached and through which no flow occurs). The default value for diameter is zero feet, implying that the cross sectional area taken up by the hub is negligible.

FAN SPEed =

Enter this command to specify the fan speed in rpm.

FAN POWer per fan =

Enter this command to specify the fan power per fan.

FAN EFFiciency =

Enter the fan efficiency as a fraction. Default is 0.7.

FAN REDucer EFFiciency =

Enter the fan reducer efficiency as a fraction. Default is 0.92.

NUMber of FANs per bay =

Enter the number of separate fans in the air-cooled exchanger.

FOUling factor AIR (1/U units) =

Enter the fouling factor for the air-side. Default is 1E-03 1/BTU/FT²/HR/ F. Other Units allowed are 1/KCAL/M²/HR/C, 1/KJ/M²/SEC/K, 1/CAL/M²/HR/C.

Air-Cooled Exchanger Tube Commands

TUBe MATerial = number

Enter choice of tube material. (default is **CAR**bon steel)

If you cannot find the specific tube material in the [Heat Exchanger: Tube Metallurgy Table](#), enter the number for the material which has an average thermal conductivity closest to the desired material.

- 1 **CAR**bon steel
- 2 **ADM**iralty brass
- 3 **STA**inless steel 304
- 4 **ALU**minum
- 5 **MON**el
- 6 **RED** brass
- 7 **COP**per
- 8 **COP**per nickel 90/10
- 9 **COP**per nickel 70/30
- 10 **NIC**kel
- 11 **TIT**anium
- 12 **ALLO**y 825
- 13 **CAR**bon **MOL**y Steel
- 14 **STA**inless steel 214
- 15 **GLA**ss
- 16 **PVC**

TUBe INSide DIAMeter (L units) =

Enter the inside diameter of the tubes. If no value is entered, it will be calculated, when TUBe BWG is specified.

TUBe OUTside DIAMeter (L units) =

Enter the outside diameter of the tubes. Default is 0.75 inches.

TUBe BWG =

Enter the Birmingham Wire Gauge for tube wall thickness. Default is 12.

TUBe WALl thickness (L units) =

Enter the wall thickness of the tubes. If no value is entered, the program will calculate it.

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TUBe LENGth (L units) =

Enter the length of the tubes. Default is 16 feet.

TUBe PITch (L units) =

Enter the tube pitch. Default is 0.9375 inches.

TUBe PASSes is also used by the rating calculation. The default value for the number of **TUBe PASSes** is one. Entry of a value for this command affects both calculations.

TUBe PASSes =

Enter the number of tube passes per shell. Default is 1.

TUBe LAYout =

Enter your choice for tube layout. Options are

- 90**-Square (default)
- 30**-Rotated Triangular
- 45**-Rotated Square
- 60**-Triangular.

FOUling factor of TUBe (1/U units) =

Enter the fouling factor for the tubes. Default is 0.001 1/BTU/FT²/HR/ F. Other Units allowed are 1/KCAL/M²/HR/C, 1/KJ/M²/SEC/K, 1/CAL/M²/HR/C.

NUMBER of TUBes per bundle =

Enter the number of tubes per bundle of the air-cooled exchanger. Default is 228.

NUMBER of tube ROWs per bundle =

Enter the number of tube rows per bundle of the air-cooled exchanger. Default is 1.

Air-Cooled Exchanger Command Summary

Command Details

TEMperature **HOT CH**ange (T units) =
TEMperature **OUT HOT** stream (T units) =
TEMperature **APPRO**ach **HOT** side (T units) =
TEMperature **OUT AIR** stream (T units) =
TEMperature **AIR CH**ange (T units) =
DUTy (H units/ t units) =
AIR FLOW rate (Q units/ t units) =

Calculation Commands

RATing on
TYPE of service =
DRAft **TYPE** of air cooler =
U-Method =
UFActor =
AREa (L² units) =
NUMBER of **PAR**allel bundles =
NUMBER of **BUND**les per bay =

Fan Commands

FAN DIAmeter (L units) =
Fan **HUB DIA**meter (L units) =
FAN SPEed =
FAN POWer per fan (Power units) =
FAN EFFiciency =
FAN REDucer **EFF**iciency =
NUMBER of **FAN**s =
FOUling factor **AIR** (1/U units) =

Optional Command Details

TEMperature **AIR IN** (T units) =
PREssure **OUT HOT** (P units) =
PREssure **OUT AIR** (P units) =
DELta **PRE**ssure **HOT** (P units) =
DELta **PRE**ssure **AIR**(P units) =
Q-T

Fin Commands

FIN MATerial =
FIN HEIght (L units) =
FIN THickness (L units) =
FIN SHApe =
NUMBER of **FIN**s **PER** tube length (1/L units) =

Tube Commands

TUBE MATerial =
TUBE THErmal **CON**ductivity (H units/t units/L units/T units) =
TUBE INSide **DIA**meter (L units) =
TUBE OUTside **DIA**meter (L units) =
TUBE BWG =
TUBE WALl thickness (L units) =
TUBE LENgth (L units) =
TUBE PITch (L units) =
TUBE PASSes =
TUBE LAYout =
FOUling factor of **TUB**e (1/U units) =
NUMBER of **TUB**es per bundle =

NUMBER of tube ROWs per bundle =

Air-Cooled Exchanger Step by Step

Air-Cooled Exchanger: Step 1

Enter all the information at the right to uniquely define the module and its connections to the rest of the flowsheet. Equipment name and connectivity (ALL are required).

Equipment module identifier	AIRC
Equipment number	Assigned equipment flowsheet number
Equipment name	User choice - up to 16 characters
Inlet stream(s)	Upto 2 streams
Outlet stream(s)	Upto 2 streams

Air-Cooled Exchanger: Step 2

Enter the module description. The module can be used in either of the two ways:

- Basic air-cooled exchanger without rating can be performed for both single and two-stream exchangers. For a single stream exchanger, air flowrate will be calculated (when not specified) and two specifications (one from the air side and one from process side) can be met. For a two-stream exchanger, one specification is met from the air and process side specifications. (please see Air-Cooled Exchanger Command Details & Air Cooled-Exchanger Optional Commands)
- Air-Cooled Exchanger Rating can be done for a single-stream and a two-stream exchanger types. For a single stream exchanger, air or process stream specifications (one) can be met when geometry (physical data on fin, fan, and tubes) and inlet process conditions are fully specified. For a two-stream exchanger, the specified geometry calculates the air and process outlet conditions along with the estimated fan horsepower. Airside heat transfer and pressure drops are calculated from general correlations.

1. Air-Cooled Exchanger Single Stream Specifications (rating off)

Total of TWO specifications are needed from the list below:

ONE process stream specification from below

Enter the estimate or specified change in temperature for the hot side. **TEM HOT CHA** (T units) =

Enter the estimate or specified outlet temperature of the hot side (gives up heat) **TEM OUT HOT** (T units) =

Enter temperature approach between air stream inlet and process stream outlet. **TEMperature APProach HOT** side (T units) =

Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger. **DUTy** (H units/ t units) =

ONE air stream specification from below

Enter the estimate or specified outlet temperature of the air (absorbs heat) **TEM OUT AIR** (T units) =

Enter change in temperature of the air stream between inlet and outlet. **TEM AIR CHA**ng (T units) =

Enter this command to specify the air flowrate for the air-cooled exchanger, if utility fluid is used. **AIR FLOW** rate (Q units) =

2. Air-Cooled Exchanger Single Stream Specifications (rating on)

When rating is required by the user for a single stream air-cooled exchanger (air flow rate is unknown), the following specification options can be used.

One among the following specifications can be met provided all geometry specifications from Air-Cooled Exchanger Rating section are also specified.

Enter this command to specify the fan power per fan.	FAN POWER per fan =
Enter the estimate or specified change in temperature for the hot side.	TEM HOT CHA (T units) =
Enter the estimate or specified outlet temperature of the hot side (gives up heat)	TEM OUT HOT (T units) =
Enter temperature approach between air stream inlet and process stream outlet.	TEMperature APProach HOT side (T units) =
Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger.	DUTy (H units/ t units) =
Enter the estimate or specified outlet temperature of the air (absorbs heat)	TEM OUT AIR (T units) =
Enter change in temperature of the air stream between inlet and outlet.	TEM AIR CHA ng (T units) =
Enter this command to specify the air flowrate for the air-cooled exchanger, if utility fluid is used.	AIR FLOW rate (Q units) =

3. Air-Cooled Exchanger Two Stream Specifications (rating off)

A two stream exchanger is defined as an exchanger with both the process and the air streams specified with temperature, pressure, and flow. One specification from the list below for the air (or) process side stream will be met. The specifications are:

Enter the estimate or specified change in temperature for the hot side.	TEM HOT CHA (T units) =
Enter the estimate or specified outlet temperature of the hot side (gives up heat)	TEM OUT HOT (T units) =
Enter temperature approach between air stream inlet and process stream outlet.	TEMperature APProach HOT side (T units) =
Enter the desired enthalpy change or duty available for the HOT side of the air cooled exchanger.	DUTy (H units/ t units) =
Enter the estimate or specified outlet temperature of the air (absorbs heat)	TEM OUT AIR (T units) =
Enter change in temperature of the air stream between inlet and outlet.	TEM AIR CHA ng (T units) =

4. Air-Cooled Exchanger Two Stream Specifications (rating on)

A two stream exchanger is defined as an exchanger with both the process and the air streams specified with temperature, pressure, and flow. When the rating is desired the specified geometry from the Air-Cooled Exchanger Rating section will decide the air and process outlet stream temperatures, along with the calculations for heat exchanged, pressure drops, and the fan horsepower.

There no specifications required for an Air-Cooled Two Stream Exchanger with rating.

Air-Cooled Exchanger: Step 3

Optional Commands

Enter the inlet temperature for the air stream. If not entered default ambient temperature will be used. Default of TEM perature of AMB ient is 77F.	TEM perature AIR IN (T units) =
--	---

Enter the desired discharge pressure for the hot stream. Defaults to feed inlet pressure or frictional delta pressure if	PRE OUT HOT (P units) =
--	--------------------------------

RATing is turned on.

Enter the desired discharge pressure for the air stream.
Defaults to feed inlet pressure or frictional delta pressure if
RATing is turned on.

PRE OUT AIR (P units) =

Enter the desired change in pressure across the exchanger
for the hot side stream.

DEL PRE HOT (P units) =

Enter the desired change in pressure across the exchanger
for the air stream.

DELta PRE AIR(P units) =

Enter this command to have duty versus temperature curves
plotted for heat exchangers.

Q-T

The Q-T table and plot are useful tools for evaluating
exchanger design. These curves are based on end-point
temperature results and counter current flow. Since air
coolers have cross flow, the minimum temperature approach
will not be accurate and may actually show cross-overs
which DO NOT actually exist. In addition, bubble points and
dew points are marked when vaporization or condensation
occurs for hot streams.

Air-Cooled Exchanger: Step 4

Enter the required specifications and options for Air-Cooled Exchanger rating.

Air-Cooled Exchanger rating options

(enter the following required command).

Air-Cooled Exchanger Rating ON

RAT

Calculation Commands

This is the type of service performed by the air-cooled
exchanger. If the choice is NOT entered flash of phase
condition in and out determines which type of air-cooler is
chosen.

TYPE of service =

TWO choices are available:

- 1 (default) Cooler, single phase, process side
- 2 Condenser, two phase, process side

This is the draft type of air-cooled exchanger.

DRAft TYPE of air cooler =

TWO choices are available:

- 1 (default) forced draft coolers.
- 2 for induced draft coolers

This is the calculation method employed for the calculation
of overall heat transfer coefficient for each stream. THREE
choices are available:

U-M = method

- 1 uses the average difference between the wall and
the fluid temperature. This is normally the most
stable method.
- 2 uses an average cube root mean temperature
difference between wall and fluid.
- 4 log mean temperature difference between wall and
fluid.

Enter this command to adjust the Overall Heat Transfer
Coefficient. It provides a "de-rating" factor for each stream
that will be multiplied with the calculated heat transfer
coefficient. The default is 1.

UFA =

Enter this command to specify the total finned surface area
of the air-cooled exchanger. If number of tubes is specified,
area can be calculated from tube geometry (given or
defaulted), then the calculated area overrides the AREa (if
given).

AREa (L2 units) =

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Enter the number of bundles in parallel. This is the total number of bundles of the air-cooled exchanger. The default is 1.

NUMBER of PARallel bundles =

Enter the number of bundles per bay. This is the number of bundles per bay of the air-cooled exchanger. The default is 1. **Note:** The number of bays is calculated as the ratio of number of parallel bundles to number of bundles per bay.

NUMBER of BUNDles per BAY =

Fin Commands

Enter the choice of fin material. (default is **ALU**minum)

FIN MATerial =

Enter this command to specify the height of the air cooler fins. Calculated from the outside diameter of the pipe and fin (Fin height = 1/2 fin outside dia - 1/2 pipe outside dia). Default is 0.626 inches.

FIN HEIght (L units) =

Enter this command to specify the thickness of air cooler tube fins. The default is 0.016 inches.

FIN THickness (L units) =

Enter this command to specify the width of the fin tip. The default is 0.0 inches.

FIN TIP width (L units) =

Enter the choice of fin shape. Choices are listed below:

FIN SHApe =

STRaight (default)

EXTruded

TRIangular

EMBedded

Enter the number of fins per inch of air-cooled exchanger tube length. The default for fins/length is 132 fins per foot (11 fins per inch)

NUM FINs PER (1/L units) =

Fan Commands

Enter the diameter (from blade tip to blade tip) of the fan. The default is 7 ft.

FAN DIA (L units) =

Enter the diameter of the fan hub (i.e. the central cylinder to which the fan blades are attached and through which no flow occurs). The default value for diameter is zero feet, implying that the cross sectional area taken up by the hub is negligible.

Fan **HUB DIA (L units) =**

Enter this command to specify the fan speed in rpm.

FAN SPEed =

Enter this command to specify the fan power.. The default is in HP. **Note:** If the fan power is entered then it becomes the specification on a single stream air-cooled exchanger. (OR) The fan power will be calculated for a two stream exchanger and will override if it is specified.

FAN POWER (Power units) =

Enter the fan efficiency as a fraction. Default is 0.7.

FAN EFFiciency =

Enter the fan reducer efficiency as a fraction. Default is 0.92.

FAN REDucer EFFiciency =

Enter the number of separate fans in the air-cooled exchanger. The default is 1.

NUMBER of FANs =

Enter the fouling factor for the air-side. Default is 1E-03 1/BTU/FT²/HR/F

FOUling factor AIR (1/U units) =

Tube Commands

Enter the fouling factor for the tubes. Default is 0.001 1/BTU/FT²/HR/ F

FOUling factor TUBE =

Enter choice of tube material. (default is **CAR**bon steel)

TUBE MATerial =

Enter the average thermal conductivity of the tube material. The default is 100 BTU/HR/FT/F (English)
Enter the inside diameter of the tubes. If no value is entered, it will be calculated, when TUBE BWG is specified.

TUBE THE CON (H units/t units/L units/T units) =

TUBE INSIDE DIAMETER (L units) =

Enter the outside diameter of the tubes. Default is 0.75 inches.

TUBE OUTSIDE DIAMETER (L units) =

Enter the Birmingham Wire Gauge for tube wall thickness. Default is 12.

TUBE BWG =

Enter the wall thickness of the tubes. If no value is entered, the program will calculate it.

TUBE WALL thickness (L units) =

Enter the length of the tubes. Default is 16 feet.

TUBE LENGTH (L units) =

Enter the tube pitch. Default is 0.9375 inches.

TUBE PITCH (L units) =

Enter the number of tube passes per shell. Default is 1.

TUBE PASSES =

Enter your choice for tube layout. Default is **90**-Square. Other choices are: **30**-Rotated Triangular; **45**-Rotated Square; **60**-Triangular.

TUBE LAYOUT = number

Enter the number of tubes per bundle air-cooled exchanger. Default is 228.

NUMBER of TUBES per bundle =

Enter the number of tube rows per bundle for the air-cooled exchanger. Default is 1.

NUMBER of tube ROWS per bundle =

Air-Cooled Exchanger Examples

There are several sample flowsheets in "Chapter 9: Air Cooled Exchanger Samples - c:\designii\samples\equipment\aircoolr" of the DESIGN II for Windows Tutorial and Samples Guide.

Air-Cooled Exchanger References

1. Single Phase Tube Side Heat Transfer Coefficient (laminar & turbulent regions) and Pressure Drop: Seider and Tate., *Industrial and Engineering Chemistry (IEC)*, Volume 28 (1936)
2. Air Side Heat Transfer Coefficient: (a) Kern & Kraus, *Extended Surface Heat Transfer*, McGraw-Hill (1972) and (b) Gardner, K. A., *Trans. ASME*, 67 (1945).
3. Single Phase Tube Side Heat Transfer Coefficient (transition region): FIG 9-7 of *NGPA* (1972).
4. Gas Processors Association, "*Engineering Data Book*", Volume 1, Chapter 10, 11th edition, (1998).
5. Chenoweth et al., "*Heat Exchanger Design Handbook*", Volume 3., Hemisphere Publishing Corporation (1983).
6. Ganapathy, V., "*Applied Heat Transfer*", pg.288, 292, and 339, Penwell Books, (1982).

Chapter 4: Amine Column

Amine Column makes use of a rate model for the rigorous simulation of absorbers, flash-gas reabsorbers and regenerators used in Amine-based (MEA, DEA, MDEA, DGA, and DIPA) gas treating processes. This truly rigorous model treats the separation as a mass transfer and/or chemical reaction rate controlled process and calculates the actual separation being achieved on each tray, or group of trays without recourse to stage efficiencies or HETP data. Detailed tray construction is used in the model. This module can be used for design, modification, or optimization of rigorous amine distillation columns. The thermodynamic models used are available in Thermodynamics: Mixed Amine. With the use of the proper option, the operation of existing units can be duplicated within several percent of actual plant data.

Amine Column Features

Amine Columns are of four different types. They are ABSorber, ABSorber with side feed, REGenerator with condenser and reboiler, and REGenerator with side draw. Please see Amine Column: Types for more details. Amine Column models rigorous simulation of absorbers, flash-gas reabsorbers and regenerators used in amine-based gas treating. This truly rigorous model treats the separation as a mass transfer and/or chemical reaction rate controlled process and calculates the actual separation being achieved on each tray, group of trays or section of packing in a tower without recourse to stage efficiencies or HETP data. Detailed tray construction or packing information is used in the model.

Each column can handle external heat exchangers. Columns are permitted to have any number of changes in diameter and any column can contain more than one type of tray (valve, bubble, or sieve) or dumped packing. A single model column must contain trays or packing exclusively but if the real column contains a packed section as well as a trayed section it can be modeled as a trayed column and a packed column in series.

Amine Column accounts for column pressure drop. Column diameter can be user-specified or calculated to achieve a specified percent of flood and can be used for rating or design.

Stream data are available from the simulation for all streams within columns including all gas and liquid streams flowing between trays or at user-designated points within packed sections. Because Amine Column deals with real physical trays and real packing, the compositions, flow rates and physical properties reported are those that should actually exist at various points within the columns.

Amine Column accesses thermodynamic and physical properties data bases that allow it to rigorously model carbon dioxide, hydrogen sulfide removal and selective hydrogen sulfide removal from a wide variety of gas streams using MEA, DEA, DGA, DIPA and MDEA. There are no inherent limitations on solvent strengths or acid gas loadings.

Flowsheet

Inlet: Two inlet feed streams mandatory for ABSorber modules and one additional side feed is allowed for the second absorber module. For regenerator module only one feed is allowed.

Outlet: Up to two material streams should leave for both the absorber and regenerator modules. One sidedraw is allowed for the regenerator module only.

Tray Ordering Convention and Input Specifications

The Amine Column ordering convention is that trays are numbered from the top of the column down (not including reboiler or condenser) and that locations within packed sections are also measured by distance from the top.

There are two types of input specifications, namely, stream specifications and equipment specifications. Amine Column input is restricted to equipment specifications only. Some data are pressure of column, number of trays, pressure drop, reboiler duty, bottoms flow from reboiler, and reboiler duty are equipment specifications. Solution circulation rates are given as part of the flowsheet specifications.

Amine Column begins with the basic column and determines the existence of a reboiler and / or a condenser. If a condenser is present, its temperature is a necessary specification.

Column Types

If the column is **TRAYED**, the following specifications must be made:

- total number of actual trays.

- either pressure on one tray and pressure drop per tray (specified or calculated) or pressure on two trays. If pressure on two trays is specified, a linear pressure profile is assumed regardless of changes in tower diameter or tray geometry.

- tray type (VALve (or) BUBble (or) SIEve), spacing and weir height in each section of the column where these differ.

- number of tray passes in each section of the column where this differs

active tray area (as actual total area, actual area per pass, or percent of tower area) for each section of the column where these differ.

tower diameter (actual or as percent of flood) for each section of the column where these specifications differ.

If the column is **PACKED**, the following specifications are necessary:

total packed depth

either pressure at one depth and pressure drop per unit depth (specified or calculated) or pressure at two depths.

If pressure at two depths is specified, a linear pressure profile is assumed throughout the column regardless of changes in tower diameter and packing parameters.

for dumped packing - the nominal size, packing factor and dry area per unit volume for each section of the column where these are different.

tower diameter (actual or as percent of flood) for each section of the column where this specification differs.

For all types of columns it is necessary to specify exact column entry and exit points for all streams.

Amine Column Command Details

Amine Column: Types

Four column types are available in the Amine Column module. The correct column type selection is based on whether the column has a condenser and/or a reboiler, a side feed, and a side draw. Once the column type is selected, the number of feeds, products, and trays, can be added. Select the appropriate column type below:

ABSorber 1

Any column with no condenser and no reboiler. A liquid feed to the top tray and a vapor feed below the bottom tray are required. A vapor product from top and liquid product from bottom are needed.

ABSorber 2

Any column with no condenser and no reboiler. There are three feeds allowed to this type. A liquid feed to the top tray and a vapor feed below the bottom tray are required, a side feed at any tray between the top and bottom is allowed.

REGenerator 1

Any column with a partial condenser and a reboiler. One feed and two products, one each from top and bottom are required.

REGenerator 2

Any column with a partial condenser and a reboiler. There is one feed allowed to this column, located at any tray in the column. There are three products, top, bottom, and sidedraw. A sidedraw at any tray between the top and bottom is also allowed.

Amine Column: Required Column Description

All the commands in this section are required for all column types. The commands provide the following basic column description:

- Tray or Packed Column Sizing. See Amine Column: Tray Sizing and Amine Column: Packed Sizing
- Pressure at the top of the column
- Pressure change in the column
- Feed tray locations
- Molar product flowrates

Column Pressures

PREssure of **TOP** tray (P units) =

Enter the top tray pressure. The top tray/packed section pressure will be used as the pressure of the top product.

PREssure **DEL**ta per **TRAY** (P units) =

Enter the pressure drop from the bottom product pressure to the top tray or packed section pressure. Default is zero.

OR

PREssure **DEL**ta =

Enter the command **DPC** so that the module will calculate the pressure drop across the trays or packed section depth.

OR

PREssure BOTtom=

Enter the bottom tray pressure. The bottom tray/packed section pressure will be used as the pressure of the bottom product

Feed Tray Location

Feeds can enter on any tray or packed section in the column. The top tray is always tray one and the condenser, if present, is tray zero. The feed tray location is the tray where any liquid in the feed would go. Also if the feed is two phase at the tray pressure, then both the liquid and the vapor portion of the feed enters the feed tray.

Feeds are always adiabatically flashed at the tray/packed section pressure. If the feed pressure is less than the tray/ packed section pressure, calculations will continue but a warning message will state that a feed pump is required.

LOCation of FEEds =

Enter the tray numbers/ or packed section depth at which feeds enter the column. Entries are in top-to-bottom order separated by commas.

Example: Amine Column 2 with 5 actual trays and three feeds:

There is a feed (stream 1) into the tray 1, a feed (stream 5) to tray 4 and a feed (stream 2) to the bottom of the column. The location of the feeds would be entered as in the following command:

AMCL1 = ABS1, 1,5,2, -3, -4,

ABS

TRA=5

LOCation of FEEds = 1, 4, 6

The first feed is to tray 1, If the feed to tray 4 is two-phase, the vapor portion will go to tray 3 and the liquid portion to tray 5. The bottom liquid feed goes into the bottom tray.

Product Flowrates

PROduct rate (molar Q/t units or FRAction) =

Enter a molar flow rate for the top or bottom product and all side draw products. The product rates must be in top-to-bottom order, separated by commas. The value of either the top or bottom product rate must be coded as zero (only in the input file creation NOT for flowsheet dialogs-defaulted to zero automatically) in order to allow an accurate overall material balance. This ensures one free degrees of freedom to perform separation based on the inlet feed flow rate.

For columns without side draws, the product rate can be entered as a fraction of the total feed to the column. Simply specify FRA in the units option for this command. E.G. PRO(FRA)= 0, .5.

- NOTE:**
1. The nonzero top or bottom molar rate is used as a heat and material balance specification.
 2. The top or bottom product's molar flowrate entered as a guess on the required PROduct rate command will be used as a heat and material balance specification if REFlux ratio specification is used for a regeneration column.

Amine Column: Product Rate Specification

The PROduct rate command must always be entered and the value of either the top (or) bottom product rate estimate must be entered. The PROduct rate command is used as an initial guess (unless REFlux ratio specification is used). Enter the top or bottom product's molar flowrate as a guess on the required PROduct rate command.

PROduct (molar Q/time into or FRA)=

Enter a molar flow rate for the top or bottom product and all side draw products. The product rates must be in top-to-bottom order, separated by commas. The value of either the top or bottom product rate must be coded as zero (only in the input file creation NOT for flowsheet dialogs-defaulted to zero automatically) to allow an accurate overall material balance. This ensures one free degrees of freedom to perform separation based on the inlet feed flow rate.

For columns without side draws, the product rate can be entered as a fraction of the total feed to the column. Simply specify FRA in the units option for this command. E.G. PRO(FRA)= 0, .5. This is particularly useful for recycle problems where the total feed rate to the column may be varying.

NOTES: The top or bottom product's molar flowrate entered as a guess on the required PROduct rate command will be used as a heat and material balance specification, if REFlux ratio specification is used for a regeneration column. Side draw product rates are normally treated as specifications and not as guesses.

Amine Column: Condenser and Reboiler Specifications

NOTE: Condenser and Reboiler Specifications are only for the REGenerator column.

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REFlux ratio =

Enter the reflux to total overhead product molar ratio. The total overhead product is vapor distillate plus liquid distillate. The default reflux ratio is set at 0.15. A typical range for amine columns is between 0.1 to 2.0

NOTE: If REFlux ratio is specified then the TEMperature of CONdenser and REBoiler DUTy specification will be ignored. Also, the PROduct Flowrate guess will be used as a PROduct Flowrate specification to be met.

OR (not available but will be included)

REFlux FLOWrate (Q units/t units) =

Enter the molar, mass, or volume rate of the liquid returning to tray one from the condenser. The reflux rate sets the condenser temperature and the amount of water refluxed back to the column.

TEMperature of CONdenser (T units) =

Enter the condenser temperature. (Column types: REG1 and REG2)

PRESSure of CONdenser (T units) =

Enter the condenser outlet temperature. (Column types: REG1 and REG2)

PRESSure of REBoiler (T units) =

Enter the reboiler outlet pressure. (Column types: REG1 and REG2)

REBoiler DUTY (H units/t units) =

Enter the reboiler duty. (Column types: REG1 and REG2)

NOTES:

For the regenerator, the value chosen for REBoiler DUTy should be such that the vapor traffic is about 10% of the liquid traffic.

Calculation of Regeneration Heat Duty for Amine/ CO₂/ H₂S systems:

1. **SENSIBLE HEAT DUTY (QS)**

$QS = (\text{Amine Flowrate}) \times (\text{Amine Heat Capacity}) \times (\text{Stripping Column } \Delta T)$

2. **REACTION HEAT DUTY (QR)**

$QR = (\text{H}_2\text{S Removal Rate}) \times (\text{H}_2\text{S Reaction Enthalpy}) \times (\text{H}_2\text{S Molecular weight}) + (\text{CO}_2 \text{ Removal Rate}) \times (\text{CO}_2 \text{ Reaction Enthalpy}) \times (\text{CO}_2 \text{ Molecular weight})$

3. **VAPORIZATION HEAT DUTY (QV)**

$QV = (\text{H}_2\text{S} + \text{CO}_2 \text{ Removal Rates}) \times (\text{Overhead Steam Ratio}) \times (\text{Steam Heat of Vaporization}) \times (\text{H}_2\text{O Molecular Weight})$

4. **TOTAL REGENERATION HEAT DUTY = QS + QR + QV**

Amine Column Optional Command Details

Amine Column: Tray Sizing

The method is general for Bubble Cap, Sieve and Valve trays. All commands are needed to design the trays within the column.

TRAYS =

This is the actual number of trays in the column.

TRAY TYPE =

Three choices are available in tray types. They are VALve, BUBble, and SIEve.

TRAY SPACING (L units) =

Enter the tray spacing to be used along with TRAY WEIr height.

TRAY PASs =

Enter the number of passes usually needed to control excessive liquid gradient. Available choices are 1, 2, 3, and 4

TRAY WEIr height (L units) =

Enter the WEIr HEIght to be used along with TRAY SPACING.

TRAY AREa PERcent of TOWER =

Enter the active tray area specified as percent of the tower cross-sectional area. The active area is the tray area available for sieve or slot openings between inlet and outlet edges of the tray.

TRAY PERcent OPEN =

Enter the tray open area percent. This applies for SIEve trays only, where the open area corresponds to number and area occupied by the openings in the tray for increased vapor and liquid contact. Normally the tray open area percent is anywhere between 8 to 20 %.

TOWer DIAMeter FLOoding percent =

Enter the percent of flood for the column on each tray. Alternately, can use the tower or column actual internal diameter in feet. Specifying one calculates the other. Note that only one among the two specifications is allowed.

TOWer DIAMeter (L units) =

Enter the tower or column actual internal diameter in feet. Multiple diameters can be specified for each tray. Alternately, can use the tower diameter flooding percent. Specifying one calculates the other. Note that only one among the two specifications is allowed.

SYStem FACTor (fraction) =

Enter the system factor to specify the foaming characteristics in the column. Default is 0.85.

Amine Column: Packed Sizing

The method is general for dumped packing only. All commands are needed to design the packed sections within the column except otherwise noted in specific commands for it's alternative use.

PACKing MATerial =

Three choices are available in packing material. They are PLASTIC (1), METAL (2) and CERAMIC (3).

PACKing TYPE =

Enter the type of packed material as DUMPed per section.

PACK DEPTH PER TYPE (L units)=

Enter the packing depth per section from the top of the column. Maximum of 10 packing sections are allowed.

PACKing DRY AREA (L2/L3 units) or (1/L units) =

Enter the packing dry surface area per unit volume for each packing section. This accounts for the porous nature of the packing material and defines the amount of available active surface for adequate liquid/ vapor contact. The dimensional units are area/ volume (or) 1/ length units.

PACKing SIZE (L units) =

Enter the packing material's size per packing section.

REDISTributors DEPTH (L units)=

Enter the depth of the redistributors from the top of the column in length units. Maximum of 10 distributors are allowed. Redistributors are not connected to the section. It serves to collect the liquid running down from the wall that has coalesced at certain sections of the column and then re-distributes the liquid to establish a uniform pattern of liquid/ gas contact.

TOWer DIAMeter (L units) =

Enter the TOWer actual internal DIAMeter per section. Should not be specified if TOWer DIAMeter FLOOD is used.

TOWer DIAMeter FLOOD (percent) =

Enter either the TOWer DIAMeter FLOODing percent per section. Should not be specified if TOWer actual internal DIAMeter is used.

PACKing FACTor (1/L units) =

Enter the packing factor per section (for dumped packing). This value is not dimensionless. Both dry or wet packing factors as provided by vendors can be used. Packing factor is a function of packing type only and is equal to surface area (wetted or dry) divided by the volume available for flow (void fraction to the power of 3). Here surface area is in L2/L3 units and void fraction is dimensionless. Reference: Separation Process Principles by Seader and Henley, 2nd edition, Page 233.

SYStem FACTor (fraction) =

Enter the system factor to specify the foaming characteristics in the packed column. Default is 0.85.

Amine Column: Internal Stream Commands

Internal streams are very useful when it is required to view the results of a stream that are internal to the Amine Regenerator Column after a column has been converged. The details of streams going in and out of column components such as condenser, and reboiler are easily obtained by using these commands. Information on temperature, pressure, and flow of each component is accessed and is displayed in the stream summary and detailed stream summary sections. Note that the numbers used for these streams should NOT be on the flow sheet. Specific internal stream commands are listed below.

Condenser Internal Streams

CON STR = x, -y

Enter this command for Amine Regenerator Column where x is the internal stream number assigned to the top tray vapor going to the condenser heat exchanger and y is the internal stream number assigned to the product going to the condenser separator (reflux accumulator).

CON SEP STR = x, -y

Enter this command for Amine Regenerator Column where x is the internal stream number from the condenser heat

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exchanger to the condenser separator and y is the internal stream from the condenser separator to the top tray (reflux).

Reboiler Internal Streams

REB STR = x, -y

Enter this command for Amine Regenerator Column where x is the liquid internal stream from the bottom tray to the reboiler and y is the vapor internal stream from the reboiler to the bottom tray excluding the product.

Amine Column: Side Feeds and Draws

Up to ONE side feed for an Absorber and ONE side draw for a regenerator can be specified.

Side Feeds

One side feed is available for ABSorber module type only. All side feeds are to be specified and will be present in the Absorber initialization. Example AMCL 1=ABS, 1, 2, 3, -4, -5

Side Draws

LOCation of SId draws =

Enter the tray number location(s) for the side draw(s) in top-to-bottom order, separated by commas. Positive tray numbers indicate a liquid draw. Negative tray numbers indicate a vapor draw.

Side draw flowrates must be specified on the PROduct rate command and are normally fixed. The side draw flowrate in the PRO command will be varied only to meet PROduct side draw specifications.

Example: LOC SID = 0, -5, 10

Amine Column: Heat Transfer Correction Factor

HTC FACTor = Enter heat transfer coefficient correction factor. Default is 0.1.

Vapor Liquid Heat Transfer Coefficient correction factor for mixed amine columns that can be used to adjust the temperature profile and bulge. This factor controls what fraction of the Chilton-Colburn analogy from mass transfer data is used for the heat transfer coefficient. The default value for this factor is 0.10. The lowest allowed value is 0.05. The highest allowed value is 0.50. Increasing or decreasing this factor can move the temperature bulge up or down the column for matching the actual data in the column. Modifying the factor can also increase the instability of the column solver and may cause the column to be unstable. A separate command, without front end dialog support, is HTC GLObal = 0.5, which will override any other value and be applied to every column on the flowsheet.

Amine Column Command Summary

Column Type

ABSorber 1
ABSorber 2
REGenerator 1
REGenerator 2

Required Column Description

PREssure of TOP tray (P units) =
PREssure of BOTtom tray (P units) =
PREssure DELta =
PREssure DEL/TRay =
LOCation of FEEDs =
LOCation of SIdedraw =
PROduct rate (molar Q/t units of FRAction) =
SYStem FACTor =

Condenser and Reboiler Specifications

REFlux ratio =
REFlux FLOWrate (Q units/t units) =
TEMperature of CONDenser (T units) =
PREssure of CONDenser (T units) =
PREssure of REBOiler (T units) =
REBOiler DUTY (H units/t units) =

Internal Streams

CON STR = x, -y
CON SEP STR = x, -y
REB STR = x, -y

Tray Sizing

TRAYS =
TRAY TYPE =
TRAY PASSs =TRAY WEIr (L units)=
TRAY SPACing (L units)=
TRAY AREa PERcent TOWER (%) =
TRAY PERcent OPEN (%) =
TOWER DIAMeter FLOoding (%) =
TOWER DIAMeter (L units) =

Packed Sizing

PACKing MATerial =
PACKing TYPE =
PACK DEPTH PER TYPE (L units)=
PACKing DRY AREA (L2/L3 units or 1/L units)=
PACKing SIZE (L units) =
REDISTributors DEPTH (L units)=
TOWER DIAMeter (L units) =
TOWER DIAMeter FLOOD (percent) =
PACKing FACTor (1/L units) =

Optional Heat Transfer Correction Factor

HTC FACTor =

Convergence Technique

TOLerance =
MAXimum MATrices =

Amine Column Step by Step

Amine Column STEP 1

Enter all the information at the right to uniquely define the module and its connections to the rest of the flowsheet.
Equipment name and connectivity (ALL are required).

Equipment module identifier
Equipment number
Equipment name
Inlet stream(s)
Outlet stream(s)

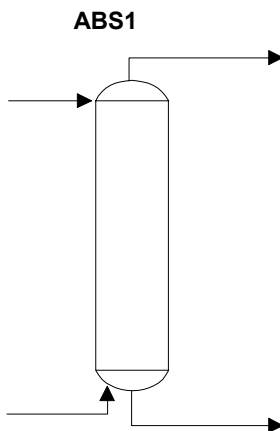
AMCL
Assigned equipment flowsheet number
User choice - up to 16 characters
Two for ABSorber. One feed for REGenerator.
Maximum of two. Sidedraw if REG2 column.

Amine Column Step 2

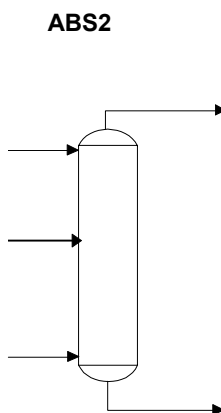
Select ONE column type from the main configurations.

There are two types of absorber column, select the one you need: ABS1 or ABS2 with side feed. If no condenser and no reboiler, THEN select absorber column type.

Absorber column

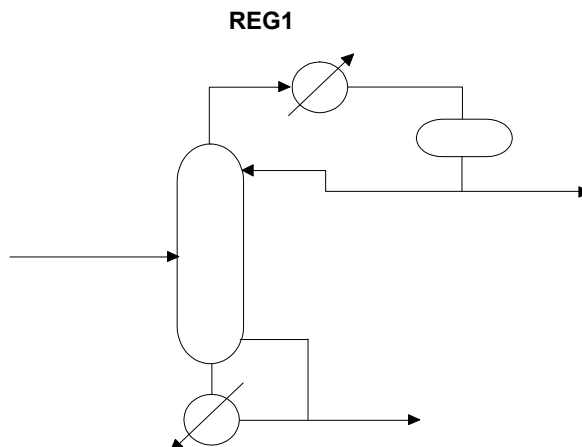


Absorber with side feed



If a partial condenser and a reboiler, THEN select Regenerator column

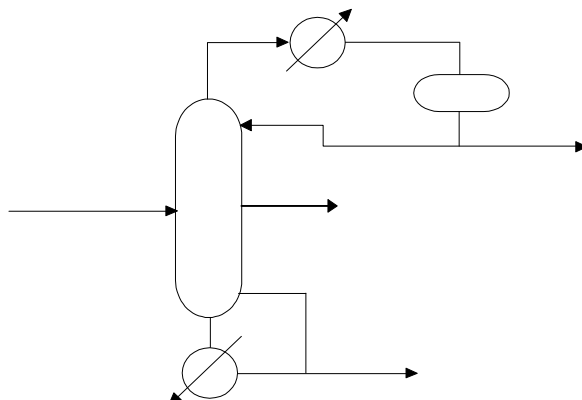
Regenerator Column



If there is a single side draw, THEN select Regenerator column Type 2

Regenerator Column

REG2



Amine Column Step 3

Enter the required column description. Required column description (enter ALL of the following)

Top tray/packed column pressure

Pressure drop from the bottom product pressure to the top tray or per depth of packing pressure. Default is zero.

Calculated pressure drop across trays or per depth of packed section (default is 0)

Enter the bottom tray/packed column pressure. The bottom pressure will be used as the pressure of the bottom product

Feed tray/packed locations (enter tray numbers or packed section separated by commas in top-to-bottom order)

Sidedraw tray/packed section location. Only one allowed for Regenerator-OPTIONAL (enter tray number or packed section at which the sidedraw is located.)

System factor to specify the foaming characteristics in the column. Default is 0.85.

Enter a molar flow rate for the top or bottom product and all side draw products. The product rates must be in top-to-bottom order, separated by commas. The value of either the top or bottom product rate must be coded as zero (only in the input file creation NOT for flowsheet dialogs-defaulted to zero automatically) to allow an accurate overall material balance.

PRE TOP (P units) =

PRE DEL

TRA

PRE DEL = DPC

PREssure **BOT**tom =

LOC FEE =

LOC SID =

SYS FAC =

PRO (molar Q units/t units or **FRA**ction) =

Amine Column Step 4

If the column is a regenerator enter the Condenser and Reboiler Options

Enter the reflux to total overhead product molar ratio. The total overhead product is vapor distillate plus liquid distillate. The default reflux ratio is set at 0.15

Enter the molar, mass, or volume rate of the liquid returning to tray one from the condenser (not available but will be included later).

Temperature out of condenser (default is top tray temperature)

Pressure out of condenser (default is top tray pressure)

Pressure out of reboiler (default is bottom tray pressure)

Reboiler duty

REFlux ratio =

REFlux **FLO**wrate (Q units/t units) =

TEM CON (T units) =

PRE CON (P units) =

PRE REB (P units) =

REB DUT (H units/t units) =

Optional Internal Streams

Enter this command for Amine Regenerator Column where x is the internal stream number assigned to the top tray vapor going to the condenser heat exchanger and y is the internal stream number assigned to the product going to the condenser separator (reflux accumulator).

Enter this command for Amine Regenerator Column where x is the internal stream number from the condenser heat exchanger to the condenser separator and y is the internal stream from the condenser separator to the top tray (reflux).

Enter this command for Amine Regenerator Column where x is the liquid internal

CON STR = x, -y

CON SEP STR = x, -y

REB STR = x, -y

stream from the bottom tray to the reboiler and y is the vapor internal stream from the reboiler to the bottom tray excluding the product.

Amine Column Step 5

Select tray sizing options.

Number of actual trays (not including reboilers or condensers, top tray = 1)

Tray type (valve, sieve, bubble)

Spacing of trays

Number of tray passes (1,2,3,4)

Weir height

Tower flooding percent each tray. Alternately, can use the tower or column actual internal diameter in feet. Specifying one calculates the other. Note that only one among the two specifications is allowed.

Tower diameter. (Multiple diameters can be specified for each tray.) Alternately, can use the tower diameter flooding percent. Specifying one calculates the other. Note that only one among the two specifications is allowed.

Tray area specified as percent of the tower or column area

Tray open area percent of the SIEVE tray

TRA =

VAL, SIE, BUB

TRA SPA (L units) =

TRA PAS

TRA WEI (L units) =

TOW DIA FLO percent =

TOW DIA (L units)=

TRA ARE PER TOW =

TRA PER OPE =

Amine Column Step 6

Select packed sizing options.

Three choices are available in packing material. They are PLASTIC (1), METAL (2) and CERAMIC (3).

Type of packed material as DUMPed per section.

Enter the packing depth per section from the top of the column. Maximum of 10 packing sections are allowed.

Enter the packing dry surface area per unit volume for each packing section. This accounts for the porous nature of the packing material and defines the amount of available active surface for adequate liquid/ vapor contact. The dimensional units are area/ volume (or) 1/ length units.

Enter the packing material's size per packing section.

Enter the depth of the redistributors from the top of the column in length units. Maximum of 10 distributors are allowed. Redistributors are not connected to the section. It serves to collect the liquid running down from the wall that has coalesced at certain sections of the column and then re-distributes to establish a uniform pattern of liquid/ gas contact.

Enter the TOWER actual internal DIAMeter per section. Should not be specified if TOWER DIAMeter FLOOD is used.

Enter either the TOWER DIAMeter FLOODing percent per section. Should not be specified if TOWER actual internal DIAMeter is used.

Packing factor per section to specify the degree of packing arrangement (for dumped packing)

PACK MAT =

PACK TYP = DUMP

PACK DEP PER TYP =

PACK DRY AREA

(L2/L3 units) or

(1/Lunits) =

PACK SIZE (L units) =

REDIST DEPTH (L units)=

TOW DIA (L units)=

TOW DIA FLOOD

(percent) =

PACK FAC (percent) =

Amine Column Step 7

Enter optional Heat Transfer Coefficient correction factor.

Heat Transfer Coefficient (default is 0.1)

Enter optional convergence control parameters.

Allowable error in tray heat and material balance (default is 1.0E-3)

Maximum number of iterations (default is 100)

Control column output

Print switch number (-2, -1, 0, 1, 2, 3) to control column output (default is 2)

HTC FAC =

TOL =

MAX ITER =

PRI SWI =

Amine Column Troubleshooting

Using the solution to another, similar problem can be a very effective means of initialization for case studies when changes in input data from case to case are not large or when the changes that are made are expected to cause relatively small changes in column performance.

This initialization procedure, where appropriate, generally results in faster convergence than any other. It is also a useful procedure to follow when difficulty is being experienced in solving a particular problem.

In such cases, the solution to the desired problem can be obtained by first solving a simpler problem, then using its solution to initialize the more difficult one. This initialization procedure should be used only when the two problems are highly correlated and very similar.

Amine Column Examples

There are several sample flowsheets in “Chapter 10: Amine Column Samples - c:\designii\samples\equipment\aminecol” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 5: Batch Distillation

Batch distillation module can be used to perform unsteady state heat and material balance calculations for Batch processes.

Batch Features

Batch distillation model provides the following features:

- Batch and Continuous Feeds
- Total or Partial Condenser
- Single or Multiple Product Collection Tanks for Each Product Draw
- Rigorous Kinetic Modeling of Reactions
- User Specified Events or Change Column Operations
- Variable Feed and Product Draw Rates
- Total Reflux Conditions Specification
- Cumulative or Instantaneous Product Composition Specifications
- Liquid Hold Up Profile Specification
- Pressure Profile Specification
- Conditional Logic Available to Control Feeds, Products and Events
- Converges Column to a large Variety of Heat and Mass Balance Specifications
- Step Functions
- Ramp Functions
- Several Integration Methods Available
- User Specified Integration Step Size
- Flexible Reporting Features
- Flexible Plotting Features

This section provides the technical information that will be required to use the Batch Distillation column. The terms and definitions are for the most part consistent with DESIGN II, however, two exceptions bear mentioning. Because of the unsteady state nature of batch distillation, streams should be considered to be tanks which serve to hold feeds or collect products. Also, keywords are grouped in specific sections within the Batch unit operation unlike other DESIGN II unit operations which have no order restriction.

Batch Event Data

At least one Event is mandatory and represents the start of the distillation. Any subsequent events begins immediately after the previous event terminates.

Batch: Required Event Commands

With the exception of PREssure and HOLdup, all of the following commands are required for every event specified. PREssure and HOLdup are required only for the first event and are optional for any subsequent events.

STArt EVENT I = event name, event type

where:

STArt EVENT

Keyword command to denote start of an event.

I

Enter number (in chronological order, starting with 1).

event name

User choice - up to 16 characters.

event type

See available event types.

Available Event Types

STEady STATE

Column operates at total reflux until steady-state condition has been reached (Dynamic Calculation).

DRAW OFF

Column operates such that a distillate product is being drawn off (Dynamic Calculation).

TOTAL REFlux

Column operates at total reflux. Steady-state calculation.

Column Conditions

PREssure (P units) i,j =

Enter one value for the Pressure on stages i through j. Command may be repeated as many times as necessary for different sections of column.

HOLdup (Q units) i,j =

Enter one value for the liquid holdup on each stage between stages i and j. Command may be repeated as many times as necessary for different sections of column. Holdup must be specified for all stages except the reboiler.

STOP WHEN (condition 1.OR.Condition...)

one of the conditions have been satisfied. Up to eight conditions for termination may be entered, separated by '.OR.'
See *Batch: Event Termination* for more information.

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NOTE: PREssure and HOLdup are mandatory for the first EVENT input only. If omitted from subsequent events, these parameters shall remain at the same values as specified in the previous event, except for HOLdup in the pot which may change due to the addition of continuous feeds or removal of products.

Batch: Heat and Material Balance Specifications

The number of specifications required depends on the event type. The following table lists the event type and corresponding number of specifications required.

Event Type	Number of Heat and Material Balance Specifications Required
total reflux until STEady STATE	1
TOTAL REFlux	1
DRAW OFF	2

Specifications Available:

VAPor to **COND**enser (Q/t units) =

Fix the total vapor flowrate passing from stage 2 to stage 1.

VAPor from **REBoiler** (Q/t units) =

Fix the total vapor flowrate passing from reboiler to bottom column stage.

CONDenser **DUTy** (H/t units) =

Enter specification for overhead condenser duty.

REBoiler DUTy (H/t units) =

Enter specification for column reboiler duty.

PRODuct **OVER**head (Q/t units) =

Enter specification for distillate product flowrate.

REFlux **RAT**io=

Enter specification for **REF**lux **RAT**io.

NOTE: All Heat and Material balance specifications will remain active in subsequent events. If different specifications are desired in subsequent events they must be entered in that event.

Batch: Continuous Feed and Side Draw Specifications

The batch distillation module provides powerful and flexible capabilities for specifying continuous feeds and side draws. The following commands describe how feeds and side draws are activated and specified. When an event terminates, all continuous feeds and side draws also terminate and they must be activated again in subsequent events if the user desires the feed or side draw to be active in the subsequent event. If the feed or side draw is reactivated in a subsequent event the flow specification does not need to be reentered, rather, it will continue as previously specified in the earlier event.

FEEds = n1 (condition1), n2 (condition2)

Enter conditions for which continuous feeds are to be active. n1, n2 represent the feeds that correspond to the nth positions in the LOC FEEd command. If no condition is specified the feed is active throughout the event.

Only one condition clause may be entered for each continuous feed.

The following variable is available for feed condition specification:

TIME (t units)

Time since the start of the event

The following logical symbols may be used in the condition clause.

.GT.

Greater than

.LT.

Less than

SIDedraws = n1(condition1), n2(condition2),....

Enter conditions for which side draws are to be active. n1,n2 represent positions in the LOC SIDedraw command. Two condition clauses may be specified per side draw.

The following variables are available for condition specification:

TIME (t units)

Time since the start of the event.

TEMperature (T units)

Temperature of the stage where the side draw is located.

LIQuid **COM**position c1,c2,...,cn

Liquid composition on the stage where the side draw is located. Composition is calculated as the sum of the specified components. C1-cn represent the positions the components occupy in the components list.

AVERage **COM**position c1,c2,...,cn

AVERage COMposition of the tank in which the side draw is being collected. Average composition is calculated as the sum of the specified components. C1-cn represent the positions the components occupy in the components list.

RECovery c1,c2,...,cn

Recovery is the total amount of the specified components collected in the tank divided by the total amount of the specified components fed to the column. C1-cn REPRESENT the positions the components occupy in the components list.

The following logical symbols may be used in the condition clause.

.GT.	Greater than
.LT.	Less than
.OR.	Or
.AND.	And

EXAMPLE:

FEEDs = 1 (TIM(HR) .LT. 1.0) , 3 (TIM(HR) .GT. 1.0)

The first continuous feed is active for the first hour only. The third continuous feed is active after the first hour only.

SIDe = 1 (LIQ COM 1.GT.0.9)

The first side draw is active only when the liquid composition of benzene on the side draw stage is greater than 0.9 (Benzene is the first component in the components list).

In addition to the above commands, the following commands are available to specify side draw flow rates or modify continuous feed conditions.

LIQuid SIDedraw (Q/t units) n

Enter a flowrate specification for the liquid sidedraw in the nth position in the LOC SIDe command. This command should be repeated for each active liquid sidedraw as indicated in the SIDedraws command.

VAPor SIDedraw (Q/t units) n

Enter a flowrate specification for the vapor sidedraw in the nth position in the LOC SIDe command. This command should be repeated for each active vapor sidedraw as indicated in the SIDedraws command.

FEED FLOW (Q/t units) n =

Enter flow rate specification for the continuous feed corresponding to the nth position in the LOC FEEd command. This command may be used to change the feed rate of a continuous feed.

FEED VAPor FRAction (molar units) n =

Enter specification for feed vapor fraction for the feed corresponding to the nth position in the LOC FEEd command. This command may be used to change the vapor fraction of the continuous feed.

FEED COMponent (Q/t) n =

This command can be used to change the continuous feed composition and flow rate. Enter component flow rates in the same order as they appear in the general section.

FEEd TEMperature (T units) n =

Enter temperature of continuous feed corresponding to the nth position in the LOC FEEd command. This command may be used to change the temperature of the continuous feed.

FEEd PREssure (P units) n =

Enter pressure of continuous feed corresponding to the nth position in the LOC FEEd command. This command may be used to change pressure of the continuous feed.

FEED ENTHalpy (H/y units) n =

Enter enthalpy of continuous feed corresponding to the nth position in the LOC FEEd command. This command may be used to change enthalpy of the continuous feed.

Batch: Optional Process Parameter Commands

The following process variables may be specified within an event. If any of these are specified they will remain specified in any subsequent event unless changed in the subsequent event.

DELta PREssure (P units) i,j=

Enter one value for the change in column pressure per stage, between stages i and j. A positive value indicates a gain in pressure, moving down column. Command may be repeated as many times as necessary for different sections of column.

DELta HOLdup (Q units) i,j=

Enter one value for the change in liquid holdup per stage between stages i and j. A positive value indicates a gain in Liquid HOLdup, moving down column. Command may be repeated as many times as necessary for different sections of column.

DUTy (H/t units) i,j=

Enter one value for the duty added/removed per stage, between stages i and j. A positive value indicates heat added to a stage, a negative value, heat removed from a stage. This command may be repeated as many times as necessary for different sections of column.

DELta DUTy (H/t units) i,j=

Enter one value for a change in duty per stage, between stages i and j. A positive value indicates a gain in heat added, moving down column. This command may be repeated as many times as necessary for different sections of column.

MURphree EFFiciency i,j=

Enter Murphree tray efficiencies for each stage between stages i and j. This command may be repeated as

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many times as necessary for different sections of column.

EXAMPLE: `DEL PRE (PSIA) 1,2 = .5`
`DUT (KCAL/HR) 2,2 = .5E6`

Batch: Variable Process Parameters and Specifications

A major capability of Batch Distillation is the ability to vary process parameters and specifications.

For each event, the process parameters and specifications (dependent variables) listed below may be input with constant values or may be varied with the *Batch STEP Function* and *Batch RAMP function*.

The dependent variables available are as follows:

(i) Process Parameters:

PREssure (P units) i,j
HOLdup (Q units) i,j
DELta PREssure (P units) i,j
DELta HOLdup (Q units) i,j
DUTy (H/t units) i,j
DELta DUTy (H/t units) i,j
LIQuid SIDedraw (Q/t units) n
VAPor SIDedraw (Q/t units) n
FEEd FLOW (Q/t units) n
FEEd VAPor FRAction (molar units) n
FEEd COMponent (Q/t units or FRA) n =
FEEd TEMperature (T units) n
FEEd PREssure (P units) n
FEEd ENTHalpy (H/t units) n

where:

i = initial stage

j = final stage

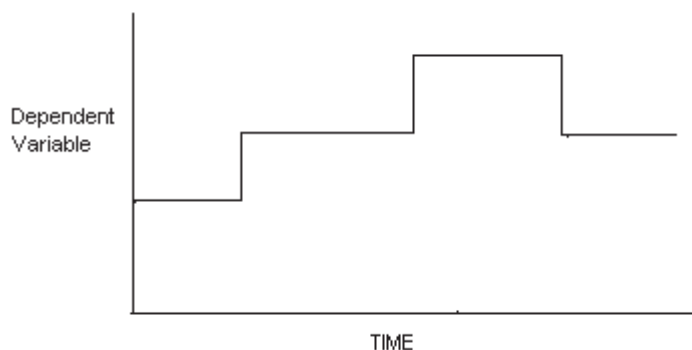
n - position of feed or side draw in the LOC FEEd or LOC SIDe command

(ii) Heat and material Balance Specifications:

VAPor to CONdenser (Q/t units)
VAPor from REBoiler (Q/t units)
CONdenser DUTy (H/t units)
REBoiler DUTy (H/t units)
PROduct OVerhead (Q/t units)
REFlux RATio

Batch: Step Function

A STEP function is used when the dependent variable changes at a number of discrete points in time, as illustrated:



Dependent Variable Vs. Time

The STEP function command has the following format:

Dependent Variable - TIME (t units)=STEP, v1, t1, v2, t2, v3, t3,...

where:

Dependent Variable Process parameter or specification from the list *Batch Variable Process Parameters and Specifications*

v1, v2, v3 etc. Dependent variable values.
t1, t2, t3 etc. Times at which STEP changes occur, time is relative to the start of the event.

EXAMPLE:

PREssure (PSIA)1,7 - TIME (HR) = STEP,16.2,0,14.6,1.0,13.1,2.0

To change a composition, the command uses the following format:

Depend variable-TIM (t units)=STEP, C11, C21, C31,..., t1, C12, C22, C32,..., t2

EXAMPLE:

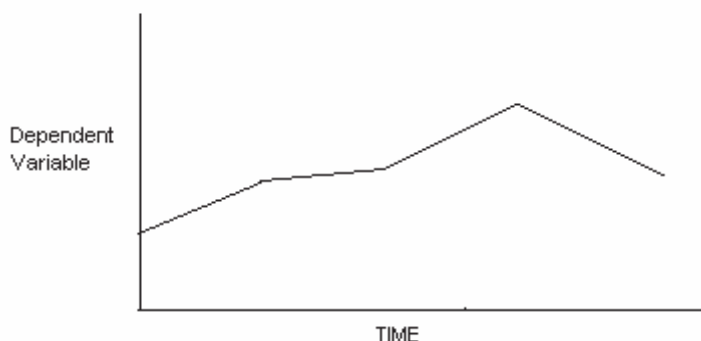
FEEd COMponent (FRAction) 1-TIME = STEP,.5,.5,1,.4,.6,2

NOTE: 1) TIME is the only independent variable available to the STEP function.
2) TIME refers to elapsed time since the start of the current event.

Batch: Ramp Function

RAMP functions may be specified as a function of the following independent variables.

- TIME (t units)
Relative time from start of current event.
- VAPor FLOWrate (Q/t units) i
Total vapor flowrate leaving stage i.
- LIQuid FLOWrate (Q/t units) i
Total liquid flowrate leaving stage i.
- STAGE TEMperature (T units) i
Temperature of stage i.
- DELta TEMperature (T units) i,j
Difference in temperature between stages i and j.



Dependent Variable Vs. Time

RAMP functions also differ from STEP functions in that the variable changes value linearly between each independent variable value as illustrated here.

The RAMP function command has the following format:

Dependent Variable - Independent Variable = RAMP, d1,i1,d2,i2,...

where:

- Dependent Variable Process parameter or specification from the list *Batch Variable Process Parameters and Specifications*
- Independent variable Variable from list above.
- d1,d2,d3 etc. Value of dependent variable.
- i1,i2,i3 etc. Values of independent variable.

EXAMPLE:

**DELta PREssure (PSI)1,7 - LIQuid FLOWrate (KGMOL/HR)2
= RAMP, 0.05, 100, 0.1, 300, 0.15, 450**

Batch: Guidelines for Variable Process Specifications.

- STEP and RAMP functions are valid only within the current event, i.e., they cannot continue into the next event. If the function is to remain active in subsequent events, the function command must be restated in all applicable event sections.
- Although the program requires information regarding PREssure and HOLdup for the distillation calculations within every event, these parameters do not need to be specified in every event sections. If none are entered, the program uses the

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values from the previous event. PREssure and HOLdup are required to be entered only for the first event. If either of these parameters are varied in a particular event using the STEP or RAMP functions and subsequent events have no entry for the same parameters, the program uses the last function-calculated value throughout all subsequent events. If the function is to remain active, it must be restated in the subsequent event inputs.

Batch: Event Termination

Up to eight conditions for termination of an event may be specified with the STOP WHEN... Command. The event terminates when any one of them is satisfied. The format of the command is:

STOP WHEN (condition 1 .OR. condition 2 .OR,...OR. condition 8)

Available variables for Stop Conditions are as follows:

TIME (t units)

Elapsed time since start of current event.

PURity SIDedraw n COM c1,c2,...,cn

Sum of flowrates of components c1,c2 etc., divided by total product flowrate for nth sidedraw in LOC SIDE Command. c1,c2,..., cn are entered as positions in the components list.

AVERAGE PURity SIDedraw n COM c1,c2,...,cn

Sum of the compositions of components c1,c2 etc. for the product tank which corresponds to the nth sidedraw in LOC SIDE Command. c1,c2,...,cn are entered as positions in the components list.

RECOVERY RATIO n COM c1,c2,...,cn

Total amount of components c1,c2 etc. collected in the product tank which corresponds to the nth side draw divided by total amount of components c1,c2 etc. in initial column charge. c1,c2,...,cn entered as positions in the components list.

FRACTION VAPorized

Ratio of total product collected in all tanks divided by initial total column charge.

TEMPerature TRAY n (t units)

Temperature of nth tray.

COMposition on TRAY n COM c1,c2,...,cn

Sum of molar compositions of components c1,c2, etc. on tray n. c1,c2,...,cn are entered as positions in the components list.

STEady STATE

Steady state distillation conditions.

Available symbols for STOP conditions are as follows:

.LT.	less than
.GT.	greater than

EXAMPLE:

```
STOP WHEN (TEM TRA 1 .GT. 101.5 .OR. STEady STATE)
STOP WHEN (AVE PUR SID 1 COM 4,6 .GT. 0.05)
STOP WHEN (FRA VAP .GT. 0.1)
```

Batch Feed Data

Batch Distillation Columns may have two types of feeds - a batch feed (initial charge) and continuous feeds. The batch feed is required, where as the continuous feeds are optional.

The continuous feeds may be specified in the GENeral section (see *Specifying A Feed Stream*) or may originate from another unit operation. One limitation that must be observed is that only one continuous feed may be located on any stage. Therefore if several streams are to be fed continuously to the same stage, they must be first combined with a MIXer.

The batch feed composition may be specified in the GENeral section or may originate from another DESIGN II unit operation. The batch feed stream only defines the batch feed composition. The batch charge is specified in one of three ways. If HOLDUP is specified for the bottom plate (pot), then the total batch charge will be the sum of the HOLDUP for the trays and the pot.

The second method of specifying the batch charge is with the TOTal CHARge command (see *Batch: Optional Configuration Commands*). Batch Distillation Columns will use the composition of the batch feed stream and the charge amount is specified with the TOTal CHARge command. If this method is being used do not specify HOLDUP for the bottom state (pot).

The third option for specifying the batch charge is with the COLlection TIME command (see *Batch: Optional Configuration Commands*). If COLlection TIME is specified, the batch charge will be the flow rate of the batch feed stream accumulated over the specified collection time period. Again, if COLlection TIME is being specified do not enter HOLDUP for the bottom stage.

TOTal CHARge and COLlection TIME may not be used together.

Batch Column Configuration

Batch: Required Configuration Commands

The following commands are all **required**:

BATch

DESIGN II keyword for Batch Distillation module.

equipment number

Assigned equipment flowsheet number.

name

User choice - up to 16 characters.

bf Inlet stream number of the batch feed.

Cf1, cf2,...

Inlet stream numbers of the continuous feeds in top-to-bottom order.

prod1, prod2,...

Outlet stream numbers in top-to-bottom order. These are coded with negative signs to indicate they are product streams.

STAges =

Enter total number of theoretical stages including any condensers and reboilers.

PARTial or **TOT**al condenser

Enter either a partial condenser or total condenser. When PARTial column type is specified, overhead product is a vapor stream. Liquid distillate is defined as side draw.

In the current release a Liquid draw cannot be located on stage number 1. Therefore a Liquid distillate for a partial condenser is defined as a liquid side draw located on stage 2. The Murphree tray efficiency for stage 2 may be set to 0.0 so that the liquid distillate is thermodynamically consistent with the liquid from stage 1. You should therefore include an extra stage when using this option.

Batch: Optional Configuration Commands

LOCation **FEEd** = i,j,....

Enter stage numbers of all continuous feeds entering column in top-to-bottom order, separated by commas. **NOTE:** Location of batch feed is not necessary since it is assumed to be charged to the bottom stage.

LOCation **SID**edraws = i,j,...

Enter stage numbers of all product draws leaving column in top-to-bottom order, separated by commas. **Note:** all products are denoted as side draws, hence overhead distillate from condenser (stage 1) would have LOC SID = 1. This command is required for a DRAW OFF event type.

TOTal **CH**arge (Q units)=

Enter the total quantity of the batch charge.

COLlection **TIME** (t Units)=

Enter time period for which the batch feed stream is to be charged to the still.

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

Batch charge temperature and pressure. If this is omitted, the batch feed temperature and pressure will be determined from the batch feed stream.

Batch Calculation Options

Due to the time dependent nature of unsteady-state distillation, the program uses an incremental time period as a basis for solving a set of differential equations. The incremental time period is known as the integration time STEP SIZE and the method used for solving the differential equations is known as the INTegration METHod. In order to provide maximum flexibility, especially for particularly difficult distillation calculations, the following commands are available and may be specified for each event. All of these commands remain active in subsequent events.

INTegration **METH**od =

- EUL - Specifies the Euler Method (default).
- RKG - Specifies Runge-Kutta-Gill method.
- IMPA - Specifies first order Euler predictor and corrector.
- IMPB - Specifies first order Euler predictor and 2nd order Adams Bashforth corrector.
- IMPC - Specifies 2nd order Adams Bashforth predictor and corrector.

STEP **SIZE** (t units)=

Enter value for Step Size. (default is .001 hours).

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MATerial BALance TOLerance =

Enter value for maximum error allowed during the integration process. (default is .1).

STEady STAtE TOLerance =

Enter value for maximum error allowed in check for STEady STAtE conditions. (default is 1x104).

VARy STEP OPTion=

s, tmin, tmax, n

where: s = scaling factor (default = 1.0)
tmin = minimum integration step size
tmax = maximum integration step size
n = number of integration steps between step size changes

Batch Reaction Data

In order to model any reactions occurring in the column, all of the following information are required.

The commands may be entered only once and in the same input section as the column configuration commands i.e. before the first **EVENT** data.

Batch: Reaction Stoichiometry

Reaction stoichiometry is specified using the following command:

$R_i = (a_1 r_1 + a_2 r_2 + \dots = b_1 p_1 + b_2 p_2 + \dots)$

where: i... = reaction number
a1,a2,... = reactant stoichiometric coefficient
b1,b2,... = product stoichiometric coefficient
r1,r2,... = reactant component ID numbers
p1,p2,... = product component ID numbers

EXAMPLE:

Reaction 1: $C_2H_6 \rightarrow C_2H_4 + H_2$

$R_1 = (1 \cdot 3 = 1 \cdot 22 + 1 \cdot 1)$

For a reversible reaction, two reactions must be specified i.e. the forward and reverse reactions.

Batch: Order of Reaction

Reactions are assumed to follow power law kinetics. The order of the reaction in a given component may be any real number (positive or negative) using the following command:

ORDER i = c1, o1, c2, o2,...cn, on

where: i = reaction number
c1, c2, cn = reactant or product component ID numbers
o1, o2,...on = order

For **example**, if Reaction 1 has a kinetic equation of the form:

$r = k [H_2]^2 [CO]$

then the order of reaction is specified as:

ORDER 1 = 1, 2.0, 48, 1.0

Batch: Frequency of Reaction

Reactions are also assumed to have an Arrhenius type expression for the rate constant. Hence, the reaction rate constant can be written.

$K = f \cdot \exp(-E/RT)$.

Care should be taken to ensure that the units of the frequency factor are consistent with the units of the rate expression. The frequency factor for all reactions are specified with the following command:

FREquency (L3 units, Molar Q units, time units) = i1, f1, i2, f2,...in, fn

where: i1, i2,...in = reaction numbers
f1, f2,...fn = frequency factors

EXAMPLE:

FREquency (M3, KGMOL, HR) = 1, 3.7E-4

NOTE: Units must be specified in order shown above.

Batch: ACTivation Energy

The activation for all reactions are specified with a single command having the form:

ACTivation energy (units) = i1, a1, i2, a2,.....in, an

where: i1, i2,....in = reaction numbers
a1, a2,....an = activation energies

EXAMPLE:

ACTivation energy (KJ/KGMOL)=1,7.5

Batch: Heat of Reaction Coefficients

Heat of reaction data must be explicitly supplied in the form of a polynomial in temperature:

HEAT of **REA**ctions (H units/Molar Q units, t units) j =

$$C1+C2*T+C3*T**2+C4*T**3+C5*T**4$$

Any coefficients which are omitted will be assumed to be zero. It should be noted that the heat of reaction is related to one molar unit of reactants being converted to product.

EXAMPLE:

HEAT of **REA**ction (KJ/KGMOL, K) 1 = 4500.,2.37,1.74E-2

Batch: Tray Reactions

Reactions only take place in the pot (or bottom tray) by default. Reactions can be caused to take place on all trays by specifying the following command.

TRAY REActions

Batch Output Specification

There are four classes of output:

- | | |
|-------------------|------------------------|
| a) History output | c) Intermediate output |
| b) Graph output | d) Final output |

Output specifications relate to events on an individual basis only. Therefore the commands described below should appear in each event input for which they are applicable. If output commands are not specified within an event, the output commands from the previous event will remain active.

Batch: History Output

History output may be used to obtain a summary of the column conditions. The user specifies the variable for which the history is desired, the time interval or number of integration steps at which the history is to be reported, and the stages for which the history is to be reported. History output is highly recommended since warning messages and data is provided which is useful when troubleshooting convergence problems.

The form of the command is:

HISTory TIME (t units) variable = time increments,s1,s2,s3,s4,s5

HISTory STEP variable = number of steps, s1,s2,s3,s4,s5

where:

s1...s5	are stage numbers - a maximum of five are allowed.
TIME	refers to elapsed time since start of current event.
STEP	refers to the number of integration steps between history prints.

The list of variables for which history output may be obtained is given below. Note that only one variable may be requested per history command, and that the variable may be reported for up to five stages in the column.

LIQuid COMposition
TEMperature
LIQuid FLOW RATE
REAction YIEld
COMponent REAction YIEld
REFlux RATio
PROduct OVERhead

NOTE: REFlux RATio and PROduct OVERhead are not related to stages, and hence stage numbers may not be supplied for

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these options.

EXAMPLE:

HIStory TIME (HR) LIQuid COMposition = 0.2,1,4,7,11,15

(will print the liquid composition on stages 1,4,7,11,15 every 0.2 hours)

HIStory STEp PROduct OVERhead = 100

(will print the total overhead product every 100 integration steps)

Batch: Graphical Output

Graphical output may be used to monitor variables as a function of time over the duration of the event. More than one graph may be requested, so that a number of variables may be tracked.

The following plot commands are available.:

PLOt TEMperature = s1,s2,s3,s4,s5

PLOt LIQuid FLOW RATE = s1,s2,s3,s4,s5

PLOt VAPor FLOW RATE = s1,s2,s3,s4,s5

PLOt REAction YIEld = s1,s2,s3,s4,s5

PLOt COMponent REAction YIEld = s1,s2,s3,s4,s5

PLOt LIQuid COMposition = s1,s2,s3,s4,s5

PLOt REFlux Ratio

PLOt PROduct OVERhead

where:

s1 - s5 stage numbers for which the variable is to be plotted.

N1... position of component in components list.

NOTE: While for the most part, variables may be plotted for up to five stages simultaneously, LIQuid COMposition, REFlux Ratio and PROduct OVERhead have a different syntax. A maximum of 5 plots are allowed.

EXAMPLE:

PLOt LIQuid COMposition = 1, 2, 5

Batch: Intermediate and Final Output

Intermediate output is printed at regular time step or integration step intervals. Final output is printed at the end of an event. Otherwise, their action is identical.

The command syntax is as follows:

PRInt INTERmediate STEp = no. of steps, option

PRInt INTERmediate TIME(t units) - time step, option

PRInt FINal = option (0 through 4, see table below, 4 is default)

The level of output required may be selected from the option table given below:

	Level 0	Level 1	Level 2	Level 3	Level 4
Temperature	-	-	yes	yes	yes
Pressure	-	-	yes	yes	yes
Vap/Liq Rates	-	-	yes	yes	yes
Vap/Liq Composition	-	-	yes	yes	yes
Enthalpy Balance	-	yes	-	-	yes
Reaction Data	-	yes	yes	-	yes
Unit Data	-	yes	-	-	yes
Product Summary	yes	yes	-	yes	yes
Material Balance Data	-	yes	-	-	yes

where:

yes denotes will be printed

- denotes will not be printed

EXAMPLE:

PRInt INTERmediate TIME(HR) = 0.5,2

PRInt FINal = 1

Composition, Vap/Liq rates and reaction data output may be printed on a molar basis, mass basis or both. To select the basis for the composition output use the following command:

PRInt BASis = MOLar (default)

 WeighT

 BOTh

This command is not relative to a specific event and therefore is not located in the event section of the input, rather it is located along with the *Batch Column Configuration*.

Batch Limitation and Assumptions

Please note the following limitations and assumptions regarding Batch Distillation calculations and output.

1. The continuous and batch feeds are always at the bubble point before integration begins. The heat duties printed in the output do not reflect the duty required to bring the material to the bubble point.
2. The component flow rates in the stream summary and detailed stream printout represent the cumulative flows into the product tanks. The temperature reported in the stream summary and detailed stream print consistent with the cumulative heat balance of the product tank.
3. The product stream flow rates for DESIGN II batch product streams are set to the entire contents of product tank flowing in a one hour time period. If a product stream is to be used to feed another down stream unit operation, the STReam MANipulator can be used to set the flow at the desired rate and a HEAt EXChanger should be used to account for any heat losses is located along with the column configuration commands (see section 3.0).

Batch Examples

There are several sample flowsheets in "Chapter 11: Batch Distillation Column Samples - c:\designii\samples\equipmnt\batch" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 6: Component Splitter

The COMponent SPLitter sends a specified fraction of each component in the feed to the first output stream (TOP). The rest of the feed is put in the second output stream (BOTtom). The temperatures of the output streams can be set to the feed temperature, bubble point, dew point, or a specified temperature. An unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest inlet pressure before the component split is performed. Two output streams **must** be coded. This module can be used to decant water, remove H₂S and CO₂ for shortcut column calculations, and for many other applications involving individual component separation.

Component Splitter Command Details

Component Splitter: Specification

RECOvery to **TOP** (Q/t units or **FRA**ction) =

Enter the flowrate or fraction of each component that goes to the first output stream. The numbers are separated by commas and must be in the order that the component ID numbers appear in the COMponent command in the GENERAL command section. FRAction is the default units option.

Component Splitter: Top Product Temperature Specification

NOTE: If none of the following commands are used, the feed temperature is used as the product temperature.

TEMperature of **TOP** (T units) =

Enter the desired temperature of the top product.

TEMperature of **TOP** is **BUB**ble point

Bubble point temperature of top product is calculated.

TEMperature of **TOP** is **DEW** point

Dew point temperature of top product is calculated.

Component Splitter: Bottom Product Temperature Specification

NOTE: If none of the following commands are used, the feed temperature is used as the product temperature.

TEMperature of **BOT**tom (T units) =

Enter the desired temperature of the bottom product.

TEMperature of **BOT**tom is **BUB**ble point

Bubble point temperature of bottom product is calculated.

TEMperature of **BOT**tom is **DEW** point

Dew point temperature of bottom product is calculated

Component Splitter Command Summary

Component Splitter Specification

RECOvery to **TOP** (Q/t units or **FRA**CTION) =

Top Product Temperature Specification

TEMperature of **TOP** (T units) =

TEMperature of **TOP** is **BUB**le point

TEMperature of **TOP** is **DEW** point

Bottom Product Temperature Specification

TEMperature of **BOT**tom (T units) =

TEMperature of **BOT**tom is **BUB**ble point

TEMperature of **BOT**tom is **DEW** point

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Component Splitter Step by Step

Component Splitter STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet streams

COM SPL

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

Two must be used

Component Splitter STEP 2

Enter the flowrate or fractions of each component to go to the first output stream. Recovery to top specification (enter corresponding to COMponent in GENeral)

Top product recovery (default is fraction)

REC TOP (Q/t units or **FRA**ction) =

Choose any of the optional specifications below. If top or bottom temperature options are not selected, the feed temperature is used as the default.

IF top product temperature option, THEN select ONE of the following:

Top product temperature

TEM TOP (T units) =

Top product dew point temperature

TEM TOP DEW

Top product bubble point temperature

TEM TOP BUB

IF bottom product temperature option, THEN select ONE of the following:

Bottom product temperature

TEM BOT (T units) =

Bottom product dew point temperature

TEM BOT DEW

Bottom product bubble point temperature

TEM BOT BUB

If thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Component Splitter Examples

There are several sample flowsheets in "Chapter 13: Component Splitter Samples - c:\designii\samples\equipmnt\comspl" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 7: Compressor

The COMPRESSOR module compresses a vapor to a specified outlet pressure or to a pressure limited by a specified work available. An unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure before compression. Either one or two output streams can be coded. If two output streams are coded, the vapor is placed in the first output and liquid in the second output. When liquid is found in the suction of the compressor, a warning message is printed. If the ENTROPY calculation is specified, a rigorous mixed-phase calculation is performed. If ENTROPY calculation is not specified, the liquid is compressed as if it were a vapor. If the vapor fraction is less than 0.5, the module shifts to a pump calculation.

Compressor Command Details

Compressor: Single Stage

WORK AVAILABLE (p units) =

Enter the available work capacity. Default is 1×10^6 HP (7.457×10^8 WA). The WORK AVAILABLE may limit the discharge pressure. Therefore, to achieve a desired work, a PRESSURE OUT guess should be entered which is greater than can be obtained with the specified WORK AVAILABLE.

PRESSURE OUT (P units) =

Enter desired discharge pressure. Default is twice the suction pressure.

PRESSURE DELTA (P units) =

Enter desired pressure change or delta pressure. Default is twice the suction pressure.

PRESSURE OUT is DEW point *and*

TEMPERATURE of DEW point (T units) =

The dew point pressure at the specified temperature is calculated and then used as the discharge pressure for the pump calculation. **Both commands must be used.** The discharge temperature is calculated by compressing the inlet stream to the dew point pressure and will not be the specified dew point temperature.

PRESSURE OUT is BUBBLE point *and*

TEMPERATURE of BUBBLE point (T units) =

The bubble point pressure at the specified temperature is calculated and then used as the discharge pressure for the pump calculation. **Both commands must be used.** The discharge temperature is calculated by compressing the inlet stream to the bubble point pressure and will not be the specified bubble point temperature.

Compressor: Multistage

If you do not enter the PRESSURE of STAGES command, DESIGN II will calculate (but not report) interstage pressures which result in equal compression ratios per stage. The PRESSURE OUT command is required, otherwise outlet pressure will be twice the suction pressure.

PRESSURE OUT (P units) =

Enter the final discharge pressure. Default is twice suction pressure.

PRESSURE DELTA (P units) =

Enter desired final pressure change or final delta pressure. Default is twice the suction pressure.

STAGES =

Enter number of stages. Maximum number of stages is ten.

PRESSURE of STAGES (P units) =

Enter the discharge pressure from each stage, separated by a comma and starting with the first stage. (e.g. PRE STA = 50, 150, 300, 600).

TEMPERATURE of INTERCOOLERS (T units) =

Enter the temperature out of interstage coolers. The discharge from each compression stage will be cooled to this temperature except for the final stage. Default is feed temperature. The interstage temperature can be specified as a fractional change from the feed temperature. A value between 1 and -1 indicates the fractional change above or below the feed temperature.

Compressor: Efficiency Commands

To simulate a compressor, you normally enter the efficiency with the following commands:

ENTROPY calculation *and*

EFFICIENCY =

Enter the adiabatic efficiency for the constant entropy calculation. Default is 0.65. To simulate a centrifugal compressor when you know the Cp/Cv ratio and polytropic efficiency, the POLYTROPIC COEFFICIENT command can be used. If you have manufacturer's curves for an existing centrifugal compressor, you should consider using the POLYTROPIC compressor

Chapter 7

module. The temperature for the POLytropic COEfficient case is calculated from the enthalpy difference due to the pressure change and work added to the system.

NOTE: Cp and Cv are calculated for each stream and printed in the Detailed Stream Report. See PRInt STReam command in CALCULATION AND PRINT OPTIONS.

POLytropic COEfficient =

Enter the polytropic coefficient (n-1)/n which is equal to (k-1)/(k* γ_p), where k=Cp/Cv and γ_p is the polytropic efficiency. Default for the coefficient is 0.22 (with n=1.282). This is the default calculation option.

and

EFFiciency =

Enter efficiency. Default is 0.72.

To simulate a compressor, you can also enter temperature out using the following commands and the isentropic efficiency of the unit module will be automatically calculated.

TEMperature OUT (T units) =

Enter desired temperature. Efficiency will be calculated.

Compressor: Method of Calculation

The equation used for compressor calculation is as follows:

$$H_p = \frac{Z_{avg} RT_1}{(n-1)/n} \left(\left(\frac{P_2}{P_1} \right)^{\frac{(n-1)}{n}} - 1 \right) \quad \text{where} \quad Z_{avg} = \frac{Z_{inlet} + Z_{outlet}}{2}$$

The temperature for *Zoutlet* is calculated using the following equation:

$$\Delta T_{ideal} = T_1 \left(\left(\frac{P_2}{P_1} \right)^{\frac{(K-1)}{K}} - 1 \right) \quad \text{where} \quad \begin{array}{l} T_2 = T_1 + \Delta T_{ideal} \\ T_2 \text{ is then rigorously calculated from the enthalpy difference} \end{array}$$

The compressor performance can be calculated by an entropy calculation method or a polytropic coefficient calculation method.

1. Entropy Calculation - This is a two step calculation. Step 1 performs a constant entropy (isentropic) calculation at T1 & P1 and T2 & P2 to determine the ideal work. Then, in Step 2, the ideal work is corrected by the isentropic efficiency to obtain the real work and the outlet temperature from an enthalpy balance.
2. Polytropic Calculation - The polytropic head is calculated by the equation for Hp above using an average Z-factor (compressibility) over a suitable increment in pressure. The polytropic coefficient is (n-1)/n = (k-1)/k*neff ; where k is the ratio of heat capacities and neff is the polytropic efficiency also over a suitable increment in pressure. The work is equal to Mass*Head / neff / 778.16 in BTUs. The temperature out is obtained by an enthalpy balance calculation as given above.

References: GPSA Engineering Data Book (11th edition, 1998, Chapter 13, pp 22 [13-22]).

Compressor: Calculate Polytropic Coefficient

The Polytropic COMPRESSor module calculates polytropic head and polytropic coefficient. The polytropic head is always calculated and the polytropic coefficient is calculated when requested with a keyword command. Both of these values are displayed in the equipment summary section of the output.

CALculate POLytropic coefficient

In the absence of this command, the polytropic coefficient defaults to 0.22.

If the ENTropy option is selected, neither the polytropic head nor the polytropic coefficient is calculated.

Compressor Optional Command Details

Compressor: Driver Commands

The program calculates the kilowatts required for electric motor drive (assuming 100 percent efficiency for the motor) for the POL COE case. The fuel gas consumption (assuming a 980 BTU/SCF fuel (8.639 x 10⁵ KJ/KGM0L) and 8000 BTU/HR/HP (3.14 x 10⁻³ KJ/SEC/WA)) will be calculated for the ENTropy case. The value will be reported in the equipment summary. You can use one of the following commands to change the default driver options:

FUEL

ELEctric DRive

If you want the steam required for steam drive to be calculated in the equipment summary, enter both of the following

commands:

STEam enthalpy IN (H/molar Q units) =

Enter the enthalpy of the steam at the inlet to the driver.

STEam enthalpy OUT (H/molar Q units) =

Enter the enthalpy of the steam at exit from the driver.

Compressor: Lost Work

TEMperature EXChange (T units) =

Enter the exchange temperature for the intercooler calculation for the LOST work analysis. Default exchange temperature is 70.3°F. This command is only used if the LOST work command has been entered in the GENeral section.

Compressor Command Summary

Single Stage Compressor

WORK AVAilable (p units) =

PREssure OUT (P units) =

PREssure DELta (P units) =

PREssure OUT is **DEW** point and

TEMperature of DEW point (T units) =

PREssure OUT is **BUBble** point and

TEMperature of BUBble point (T units) =

Multistage Compressor

PREssure OUT (P units) =

STAgEs =

PREssure of STAgEs (P units) =

TEMperature of INTERcoolers (t UNITS) =

Lost Work

TEMperature EXChange (T units) =

Efficiency Commands

ENTropy calculation and

EFFiciency = fraction

POLytropic COEfficient = and

EFFiciency = fraction

TEMperature OUT (T units) =

(Efficiency will be calculated.)

Driver Commands

FUEL

ELEctric DRive

STEam enthalpy IN (H/molar Q units) =

STEam enthalpy OUT (H/molar Q units) =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Compressor Step by Step

Compressor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet streams

COMPRE

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

One or two; if two, 1st is vapor, 2nd is liquid

Compressor STEP 2

Choose either a single or multistage compressor module.

IF single stage compressor THEN enter ONE of the following:

IF available work capacity (default is 1 million HP)

IF Outlet pressure (select ONE of the following three options)

Discharge pressure (default is twice suction)

Pressure Change or Delta (default is twice suction)

Dew point pressure at temperature

Bubble point pressure at temperature

WOR AVA (p units) =

PRE OUT (P units) =

PRE DEL (P units) =

PRE OUT DEW

TEM DEW (T units) =

PRE OUT BUB

TEM BUB (T units) =

IF multistage compressor THEN enter ALL of the following

Number of stages

Intercooler temperature (default is feed temperature)

Stage outlet pressure (enter value for every stage)

Discharge pressure (enter final discharge pressure)

STA =

TEM INT (T units) =

PRE STA (P units) =

PRE OUT (P units) =

Compressor STEP 3

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Choose the desired efficiency option.

Efficiency specification (enter ONE of the following)

Entropy - Adiabatic efficiency (default is 0.65)

Polytropic coefficient - polytropic efficiency (defaults are 0.22 and 72)

Temperature Out (Efficiency will be calculated)

IF driver options THEN select ONE of the following:

Electric motor

Fuel gas turbine

IF stream is required for your drive, enter both of the following

Steam enthalpy in

Steam enthalpy out

IF thermo is different from global (GENeral section) options THEN select:

K-value option

Enthalpy option

Density option

IF LOST work option THEN select exchange temperature for lost work (default is 70.3 F)

ENT, EFF =

POL COE =

EFF =

TEM OUT (T units) =

ELE DRI

FUEL

STE IN (H/molar Q units) =

STE OUT (H/molar Q units) =

KKE =

HKE =

DKE =

TEM EXC (T units) =

Compressor Examples

There are several sample flowsheets in "Chapter 12: Compressor Samples - c:\designii\samples\equipmnt\compre" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 8: Controller

Like all equipment modules, the CONTroller is located in the flowsheet by means of input and output stream numbers. However, the CONTroller does not alter its streams in any way; the stream out is identical to the stream in. The CONTroller can only measure stream information and cannot change it except via an equipment module.

Controller Features

Passing Information

When passing information, the CONTroller module must be located after the equipment module that calculates the information to be passed, and before the module to which the information is passed. For example, when passing work produced in an EXPander to a COMPRESSor, the CONTroller module must be located after the EXPander module. The stream out of the EXPander should be coded into the CONTroller.

Setpoint Convergence

When converging to a setpoint, the CONTroller module should be located after the equipment module that calculates the property being compared to the setpoint. The CONTroller module, when used to obtain a setpoint, changes the order of equipment calculation. After the CONTroller is calculated, calculation order returns to the equipment module where the VARied property is located. Make sure that the equipment that is varied is calculated before the CONTroller. Also you must make sure all other equipment instrumental in calculating the measured property or properties have been calculated. The equipment calculation sequence can be determined by using a CHECK INPUT command in the GENERAL command section of the input for the first run. If the calculation sequence is not satisfactory, you can change it by using the RECYCLE SEQUENCE command in the GENERAL section. See *Recycle Loops* Section.

Recycle Simulation with CONTrollers

When your simulation involves both a recycle loop and a setpoint convergence CONTroller, certain restrictions apply. A CONTroller loop is formed by the equipment whose specification is varying, the equipment or stream whose property is being measured, and the CONTroller module itself. This CONTroller loop must be either completely inside or completely outside any recycle loop. In particular, the CONTroller loop and the recycle loop must not begin or end with the same equipment in the flowsheet.

A CHECK INPUT run should be made first to determine the equipment calculation sequence and recycle streams. If the CONTroller loop is valid, the complete simulation may then be run. For this run, you should omit CHECK INPUT, include recycle stream guesses (FLO and TP in GENERAL section), and specify a maximum number of recycle loops.

You should also consider using the GENERAL section command PRINT FREQUENCY = 1. You can set the sequence of equipment calculations using the RECYCLE SEQUENCE command. See *Recycle Loops* Section.

Changing Stream Parameters

The CONTroller module by itself cannot change stream parameters - it must be used with another equipment module.

Changing Stream Pressure: Use the CONTroller with the PUMP, COMPRESSor, EXPander, or VALVe module.

Changing Stream Temperature: Use the CONTroller with the HEAT EXChanger or FIRed HEATER.

Changing Total Flowrate: Use the CONTroller with the STReam manipulator or the DIVider module.

NOTE: WARNING: If you want to vary the FLOW RATE on a DIVider module which is coded as a FRAction, be sure you have only two streams out of the DIVider. Code the second stream FRAction as zero. For example:

```
DIV 10 = SPLT, 1, -2, -3, FLOW RATE (FRA) = .5, 0
```

Nonmolar Flow Rates

Occasionally the setpoint may be on a volume basis. The CONTroller can only access flows in molar or mass units. A STReam manipulator can be used to force the measured flow to be gallons (or other volumetric units) per hour by using the MUL, FAC options. See *Stream Manipulator* section for details.

Controller Command Details

Controller Passing Information

SET X1 OF equipment =

X2 (SCALE =) FROM ES operator X3 (SCALE =) FROM ES

X1 is an Equipment Module keyword command; e.g. TEM OUT for HEAT EXChanger

equipment is the Equipment Module identifier and equipment number e.g. HEA EXC 7

X2, X3 are any calculated equipment or stream properties; e.g. CAL DUT for a HEAT EXChanger or FLO COM for a stream. X2 and X3 can also be Equipment Module keyword commands; e.g. TEM OUT for a HEAT EXChanger is a stream as identified by STR and stream number; e.g. STR 18

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ES is the Equipment Module identifier and equipment number *OR* the stream number and identifier (e.g. STR 18).
SCALE = multiplication factors used to modify X2 and X3 (Default is 1.0).
operator +(add), -(subtract), *(multiply), /(divide)

NOTE: operator and X3 are optional

Examples:

```
SET WOR AVA OF COMPRES10 = CAL WOR (SCA = 98) FRO EXP 4  
SET DUT OF HEA EXC 5 = CAL REB (SCA = 1) FRO DIS 4
```

NOTE: CONTROLLER input can only be broken after the = sign.

Controller Setpoint Convergence

VARY X1 (MIN =, MAX =, STE =, units) OF *equipment*

UNTIL X2 (SCALE =) FROM ES operator X3 (SCA =) FROM ES=
constant (SCA =, BEG =, LOO =, TOL =, units)

-OR-

X4 (SCA =, BEG =, LOO =, TOL =) OF ES

X1 is an Equipment Module keyword command; e.g. TEM OUT for HEAT EXChanger equipment is the Equipment Module identifier and equipment number e.g. HEA EXC 7

X2,X3,X4 are any calculated equipment or stream properties from Tables 1 and 2; e.g. CAL DUT for a HEAT EXChanger or FLO COM for a stream. X2, X3, and X4 can also be Equipment Module keyword commands; e.g. TEM OUT for a HEAT EXChanger constant is a desired setpoint value. Units must be specified if other than US defaults.

ES is the Equipment Module identifier and equipment number *OR* the stream number and identifier (e.g. STR 18).

SCALE = multiplication factors used to modify X2, X3, and X4 (Default is 1.0)

operator +(add), -(subtract), *(multiply), /(divide)

MINimum value = is the specified minimum value for X1

MAXimum value = is the specified maximum value for X1

STEP size = is the maximum step size to be taken when varying a specification. The initial step will be five percent of the specified step size to determine the slope and direction for the next change.

TOLERance = is the absolute difference acceptable for setpoint convergence. Default is the relative CONvergence TOLERance specified in the GENeral command section.

BEGin loop = is the process control loop iteration number at which action of the CONTROLLER is to begin. Default is first process loop.

LOOps = Maximum number of controller loops for setpoint convergence. Default is 30.

units Units must be specified where indicated for MIN =, MAX =, and STE =, and for constant if other than American defaults; e.g. ATM for pressure. See INPUT / OUTPUT UNITS Section for details.

VARY X's (MIN=, MAX=, STE=, units) of equipment

UNTIL X2 (Scale) FRO name operator X3 (scale) Fro name =

X4 (Scale=, BEGin =, LOOps =, TOL=) OF name

NOTE: X4 can also be constant, X3, operator are optional.

Examples:

```
VARY TEM OUT (MIN = 100, MAX = 200, STE = 10, C) OF HEAEXC7  
UNTIL FLO STR 18 = 100  
VARY FLORAT (MIN = .01, MAX=.99, STE = .098) OF DIV17  
UNTIL FLO STR 100/FLO STR 6 = .7  
VARY PRO1 (MIN = 500, MAX = 575, STE = 7) OF DIS 14  
UNTIL FLO COM 3 FRO STR10/FLO STR 10 =.75 (BEG = 2, LOO = 5)  
VARY FLO (MIN=0.05, MAX=1.0, STEP=0.05) OF DIV 1  
UNTIL FLO FROM STR 6=18000 (TOL=1,LOO=100,LB)
```

NOTE: CONTROLLER coding can only be broken as shown in examples.

Controller Command Summary

Passing Information

SET X1 OF *equipment* =

equipment

equipment

X2 (SCALE =) FROM or operator X3 (SCALE =) FROM or
stream stream

Setpoint Convergence

VARY X1 (MIN =, MAX =, STE =, units) OF equipment

UNTIL X2 (SCALE =) FROM equipment or operator X3 (SCALE =) FROM equipment or
stream stream =

constant (SCALE =, BEG =, LOO =, TOL =, units)

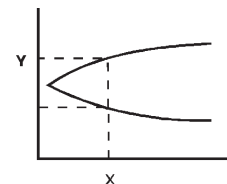
or equipment
X4 (SCALE =, BEG =, LOO =, TOL =) OF or
stream

NOTE: *Controller: Table 1. Calculated Equipment Properties* and *Controller: Table 2. Stream Properties* list the specifications available for Xi.

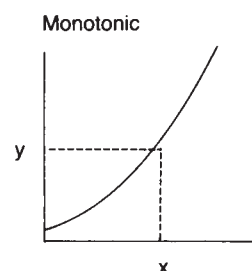
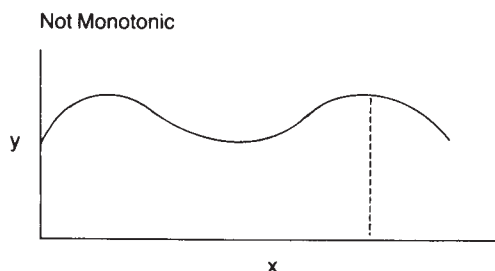
Controller Setpoint Logic

In order to use the setpoint CONTroller effectively, there are a few simple rules to keep in mind when setting up your simulation. In the discussion which follows, the independent variable is the equipment specification you are telling the program to VARY. The dependent variable is the measured value (or setpoint) you are trying to meet. The relationship between the independent and dependent variables should be direct (a change in the independent variable will cause a noticeable change in the dependent variable). This relationship has to obey certain rules.

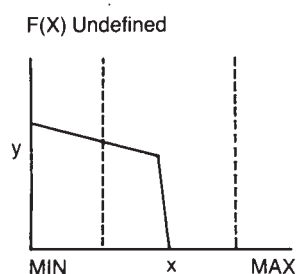
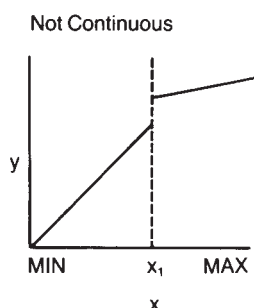
1. The measured variable, y, should have only one value for every value of the independent variable, x. The function $y = f(x)$ shown here, is an example of an inappropriate controller function that is multiple-valued with respect to x.



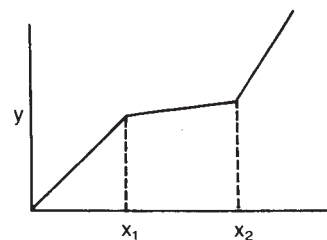
2. The controller provides more predictable behavior if y is monotonic with respect to x. In the first example below, there are several values of x for which y has the same value. In this situation the controller may not converge to the expected value of x. In the second example the measured variable is monotonic with respect to x. Appropriate choices of the MINimum and MAXimum of the independent variable will restrict the controller to a range where y is monotonic.



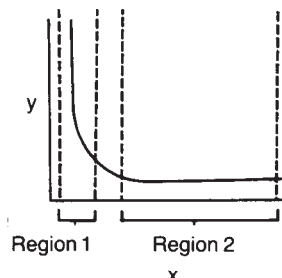
3. The measured variable, y, should be defined within the boundaries of the independent variable, x. Boundaries of the independent variable, x, are fixed with the MINimum and MAXimum specifications in the controller statement. In the first example, the measured variable, y, is discontinuous at x1. In the second example the measured variable becomes zero within the boundaries on x. This problem can be avoided by setting the boundaries to exclude the discontinuities or undesired behavior of a function.



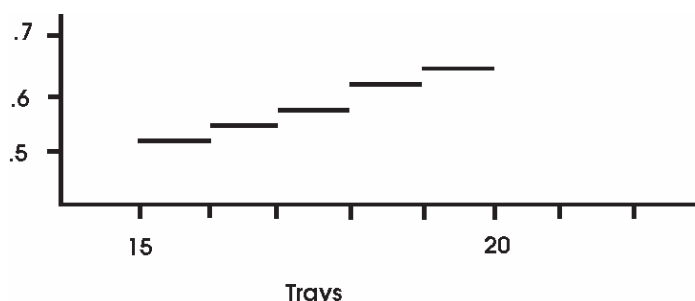
4. The slope of y , dy/dx , must be continuous. In the example shown here, the measured variable, y , is continuous but not smooth with respect to the independent variable, x . Therefore, the slope at x_1 and x_2 will be discontinuous. MINimum and MAXimum must be chosen to prevent the CONTroller from seeing these points.



5. Very large changes in y with respect to a small change in x or a very small change in y with respect to a large change in x can cause convergence problems for the CONTroller. In the example shown here, both types of behavior are demonstrated. In region 1, small values of the STEP size are required with narrow boundaries on x . In region 2, a large STEP size is required with wide boundaries on x .



6. An example of setpoint controller coding where y is neither monotonic nor a function is VARY TRAYS in a DISTillation column to meet a desired product composition (for example, purity of propane in the bottom product). DESIGN II only accepts integer values for TRAYS. The calculated product composition may result in a new value of 16.6 trays which will be interpreted as TRAYS = 16. Careful selection of step size (STEP size of 2 or 3 trays) and TOLERance (use looser tolerance than default) may allow convergence.



NOTE: When trays are added or removed from a column calculation, the current feed location(s) may no longer be optimum. Since feed tray location is counted from the top, the change in number of trays primarily affects the stripping section, not the rectifying section.

The CONTroller uses a bounded secant method to solve for the independent variable, x . The MINimum and MAXimum you specify for the CONTroller determine the range of values for x . The STEP size you specify limits (or bounds) the change in the x value from one controller iteration to the next. The secant method approximates $F(x)$ by drawing a line between the current and previous values of $F(x)$ (the measured variable), then solves for the x -intercept of the line. This new x is used as the new specification value in the assigned equipment unless the change in x is greater than the maximum STEP size. In that case, the new x will be computed by adding (or subtracting) the maximum STEP size to the current value of x . This process continues until one of the three following conditions is met:

1. The CONTroller has converged (measured value matches the setpoint within the specified tolerance),
2. The MAXimum or MINimum value specified for x has been reached, or
3. The specified number of LOOps has been calculated without reaching convergence (default is 10 loops).

Controller Review of the Output

The controller output includes values labeled NEW F, OLD F, MEASURED VARIABLE, and SETPOINT. NEW F is the updated value of the independent variable (the specification being varied) to be used for the next loop and OLD F is the value of the independent variable used to obtain the MEASURED VARIABLE for the current iteration. SETPOINT is the desired value for the measured variable (the controlled variable).

The following output is from a controller module setting a temperature ratio (temperature of one stream divided by the temperature of another stream) to 1.0 by varying the flowrate from a divider module. In the printout F refers to the flow rate and VARIABLE to the temperature ratio.

```

NOW CALLING EQUIPMENT 6 + CONT (CONT) +
P.R. KVALUES P.R. ENTHALPY P.R. DENSITY
+++ CONTROL BLOCK 6
NEW F - 0.6680 OLD F -0.703999877
MEASURED VARIABLE 0.97119796 SETPOINT 1.0000000
    
```

Controller Troubleshooting

When the MAXimum or MINimum value for the independent variable has been reached without meeting the setpoint, review the output. Determine if changes in the independent variable (labeled as OLD F and NEW F in your output) are causing the value for the measured variable to move closer to the setpoint. If so, change the appropriate limit (if feasible) and start the calculations over, using the latest value for NEW F.

If a CONTroller calculation requires more than 30 iterations to converge (and is not oscillating between two values), you should consider changing either the initial value for the independent variable (the value you enter for the equipment specification which is being VARied) or the STEP size. Ideally the initial value for the independent variable will be halfway between the MINimum and MAXimum values specified for the CONTroller. Usually the STEP size will be set equal to MAXimum-MINimum divided by 30 (or the number of LOOps you specify).

Oscillation of NEW F and OLD F between two values for several iterations may indicate either a discontinuity or a process restraint. Review results to determine which is the case, make appropriate adjustments to MIN, MAX or STEP and rerun. Oscillation may also occur if calculations reach either a local maximum or minimum without meeting your setpoint. Some change in process conditions will be required.

Controller Step by Step

Controller STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier	CONT
Equipment number	Assigned equipment number
Equipment name	User choice - up to 16 characters
Inlet stream	One only
Outlet streams	One only

Controller STEP 2

Enter the information shown below to set an equipment specification. To vary an equipment specification go to STEP. Setting an equipment specification:

To use this option, you need to define terms in the CONTroller "SET" equation:

SET X1 = X2 (SCALE =) operator X3 (SCALE =)

X1 is the equipment specification to be set (e.g. REFlux ratio, TEMperature OUT, LOCation for FEEd, DUTy, etc.)

X2,X3 are the equipment specifications, calculated results, or stream properties in *Controller Table 1. Calculated Equipment Properties for Controller* and *Controller Table 2. Stream Properties* (TEMperature, REFlux, FLOWrate, etc.). The operator and X3 are optional.

SCALE multiplication factors used to modify X2 and X3 (default is 1.0)

operator is + (plus), - (minus), * (multiply), or / (divide)

Input format

SET X1 OF equipment =

X2 (SCALE =) FROM

equipment	or	equipment
stream	or	stream

 operator X3 (SCALE =) FROM

equipment	or	equipment
stream	or	stream

NOTE: controller module command lines for setting equipment specifications can only be broken as shown above.

Controller STEP 3

Enter the information below for setpoint convergence.

To use this option, you need to define terms in the CONTroller "VARY" equation:

VARY X1 UNTIL X2 (SCALE =) operator X3(SCALE =)

X4 (SCALE =)
or
constant (SCALE =)

X1 is the equipment specification to be varied

x2, x3, x4 are equipment specifications, calculated results, or stream properties in *Controller Table 1. Calculated Equipment Properties for Controller* and *Controller Table 2. Stream Properties* The operator and X3 are optional.

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SCALE multiplication factors used to modify X2, X3, X4 or constant (default is 1)
operator is + (plus), - (minus), * (multiply), or / (divide)

Input format

VARY X1 (**MIN** = , **MAX** = , **STE** = , units) **OF** equipment

UNTIL X2 (**SCALE** =) **FROM** ^{equipment}
or ^{equipment}
stream **operator** X3 (**SCALE** =) **FROM** ^{equipment}
or ^{equipment}
stream

X4 (**SCALE** = , **BEGIN** control loop = , **LOOPS** = , **TOLERANCE** = , units)
or
constant (**SCALE** = , **BEG** = , **LOO** = , **TOL** = , units)

NOTE: controller module command lines for setpoint convergence can only be broken as shown above.

Controller Table 1. Calculated Equipment Properties

The following list of commands provides the CONTROLLER module access to calculated information for the various equipment modules.

Rigorous Column - DIS

CALculated **COND**enser duty
CALculated **GL**itsch **PER**cent flooding
CALculated **REBO**iler duty
CALculated **REF**lux
CALculated **TEM**perature **TOP** (product)
CALculated **TEM**perature **BOT**tom (stage)
CALculated **MAX**imum **DIA**meter
CALculated **PRO**duct rate

Pumps, Compressors, & Expander - PUMP, COMPRE, EXP

CALculated **WORK** for the machine (positive for EXP)
CALculated **ELEC**trical power usage
CALculated **FUE**l gas consumption
CALculated **STE**am consumption
CALculated **WATER** for cooling for multistage compressor

Fired Heater - FIR

CALculated **FUE**l gas consumption
CALculated **HEAT ABS**orbed
CALculated **DUTY**

Heat Exchanger - HEA EXC

CALculated **ARE**a
CALculated **DUTY**
CALculated **LMTd** (corrected log mean temperature difference)
CALculated **WATER** flowrate for water cooled exchanger
CALculated **EFFECTIVE ARE**a of the exchanger per the rating calculations
CALculated **ACTUAL ARE**a of the exchanger per the rating specifications

Reactor - REA

CALculated **DUTY**

LNG Heat Exchanger - LNG

CALculated **ARE**a of the nth input stream
CALculated **DUTY** of nth input stream; n is the position of the tubeside stream on the equipment command
CALculated **LMTd** of the nth input stream, where n is defined above
CALculated **MIX TEM**perature for shellside feed after tubeside recycle
CALculated **TOTAL** of individual **ARE**as
CALculated **TOTAL** of individual **DUTIES**

Polytropic Compressor - POL

CALculated **SPEED**
CALculated **SUCTION VOLUME**

Shortcut Fractionator - SHO

CALculated **DUTY** of **COND**enser
CALculated **DUTY** of **REBO**iler
CALculated **FEED TRAY** location from the top
CALculated **MINIMUM REF**lux ratio of infinite stages
CALculated **REF**lux ratio
CALculated **STAGES** (theoretical)
CALculated **MINIMUM** stages

Stream Manipulator - STR

CALculated value per **MOLE**
CALculated value per **SCF**

NOTE: For equipment module specifications having multiple values, you must enter a number indicating the position of that specification. e.g. PRO 2 FROM DIS 10.

The sign convention for reported duties is as follows: heat added to the stream will be reported as positive duties, heat removed from the stream will be reported as negative duties. Also, work created by an expander will be reported as positive, and work required by the compressor or pump will be reported as negative work.

Controller Table 2. Stream Properties

The following commands are used to identify stream properties to the CONTROLLER.

ENTHalpy of the stream

ENTRopy of the stream

FLOWrate of stream

FLOWrate of **COM**ponent i in the stream, where i is the component identification number

FLOWrate of **COM**ponent **MAS**s i in the stream, where i is the component identification number

FLOWrate **MAS**s of **COM**ponent i in the stream, where i is the component identification number

FLOW COMPONENT FRACTION *i* in the stream, where *i* is the component identification number

PREssure of the stream

TEMperature of the stream

VAPor **FRA**ction of the stream

VAPor **MASS FRA**ction of the stream

REID VAPor pressure of a stream (for which the REID vapor pressure calculation is requested in the **GEN**eral section)

NOTE: Either **molar** or **mass** quantity over time flowrate units can be used for the stream flowrates.

The above overall **FLOW**rate of stream, **FLOW**rate of **COMP**onent *i* and **FLOW COMPONENT FRA**ction *i* in the stream commands, are by default in molar units. For mass units, the same commands can be used as shown in the two sample controller codings below:

```
VARY FLO (MIN=0.05, MAX=1.0, STEP=0.05) OF DIV 1
UNTIL FLO FROM STR 6=18000 (TOL=1, LOO=100, LB)
```

and

```
VARY FLO (MIN=0.05, MAX=1.0, STEP=0.05) OF DIV 1
UNTIL FLO COM 49 FROM STR 6=400 (TOL=1, LOO=100, LB).
```

Controller Table 3. Variables Available to SET and VARY

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Controller: SET/VARY-UNTIL Variables for Add Module

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Air Cooled Exchanger

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
TEMperature HOT CH ange	Temperature change for the hot side	R
TEMperature OUT HOT side	Temperature out of hot side	R
TEMperature APPR oach HOT side	Temperature approach of hot side	R
TEMperature OUT AIR stream	Temperature out of air side	R
TEMperature AIR CH ange	Temperature change for the air side	R
DUTY	Duty of aircooler	BTU/HR
AIR FLOW rate	Air flowrate	LBMOL/HR
FAN POWER per fan	Fan power	HP

Controller: SET/VARY-UNTIL Variables for Amine Column

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Batch Distillation

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Component Splitter

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A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
REC TOP(i)	Flowrate or fraction of "ith" component in 1st outlet	*
TEM BOT	Temperature of second outlet	R
TEM TOP	Temperature of first outlet	R

*Default is molar fraction, otherwise flow units as specified in input.

Controller: SET/VARY-UNTIL Variables for Compressor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
CAL ELE	Calculated electricity usage	KW
CAL FUE	Calculated fuel gas usage	SCF/HR
CAL STE	Calculated steam usage	LB/HR
CAL WAT	Calculated cooling water (multistage)	GAL/HR
CAL WOR	Calculated work required (always negative)	HP
EFF	Efficiency	----
POL COE	Polytropic coefficient	----
PRE OUT	Final discharge pressure	PSIA
PRE STA (i)	Discharge pressure for stage (i)	PSIA
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 DEW	Temperature for spec PRE OUT at DEW PT	R
TEM INT	Temperature interstage cooler	R
WOR AVA	Available work	HP

Controller: SET/VARY-UNTIL Variables for CSTR

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
<u>CSTR</u>		
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Depressurizer

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
<u>DEPressuring</u>		
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Distillation

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
DEL	Pressure drop through column	PSI
CAL CON	Calculated condenser duty	BTU/HR
CAL GLI PER	Calculated Glitsch Percent tray flooding	%
CAL MAX DIA	Maximum diameter from Smith-Dresser-Ohlswager tray sizing	FT
CAL PRO (i)	Calculated "ith" product	*
CAL REB	Calculated reboiler duty	BTU/HR
CAL REF	Calculated reflux ratio	----
CAL TEM TOP	Calculated temperature for top product	R
CAL TEM BOT	Calculated temperature for bottom product	R
DUT CON	Specified condenser duty	BTU/HR
DUT INT(i)	Intercooler duty of "ith" tray	BTU/HR
GLI PER	Specified Glitsch flooding percent for the column	%
HEA (i)	Heat added/removed from "ith" heater/cooler	BTU/HR
PRE CON	Condenser pressure	PSIA
PRE TOP	Top tray pressure	PSIA

PRO (i)	Rate for "ith" product	LBMOL/HR
REB	Specified reboiler duty	BTU/HR
REF	Reflux ratio	----
REF FLO	Reflux flowrate	LBMOL/HR
TEM BOT	Guess for bottom product temperature	R
TEM CON SUB	Degrees of subcooling for total condenser	R
TEM CON	Condenser temperature	R
TEM INT (i)	Temperature for "ith" intercooler	R
TEM REB	Specified reboiler temperature	R
TEM TOP	Guess for top product temperature	R
THE	Mole fraction vaporized from thermosiphon reboiler	----
RAT BOT i, j	Molar ratio of component i to component j in bottom	----
RAT TOP i, j	Molar ratio of component i to component j in top	----
RAT SID i, j, n	Molar ratio of component i to component j in side draw n	----
REC BOT i	Molar flow of component i in bottom	LBMOL/HR
REC TOP i	Molar flow of component i in top	LBMOL/HR
REC SID i, n	Molar flow of component i in side draw n	LBMOL/HR
PUR BOT i	Molar fraction of component i in bottom	----
PUR TOP i	Molar fraction of component i in top	----
PUR SID i,n	Molar fraction of component i in side draw n	----
TOL	Tolerance for column convergence	----

*Default is lbmol/hr; if FRA specified, value is fraction of total feed.

**RATio, RECover, PURity, and TOTal PROduct specification only.

Controller: SET/VARY-UNTIL Variables for Divider

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
FLO RAT i	Flowrate of "ith" outlet	*
*Default is molar fraction; otherwise flow units as specified by user in input.		
*LBMOL/HR, LB/HR, OR GAL/HR depending upon input being molar, mass or volumetric units		

Controller: SET/VARY-UNTIL Variables for Equilibrium Reactor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Expander

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
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 (produced)	HP
EFF	Adiabatic efficiency	----
PRE OUT	Final discharge pressure	PSIA

Controller: SET/VARY-UNTIL Variables for Fired Heater

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
CAL FUE	Calculated fuel usage	SCF/HR
CAL HEA ABS	Calculated heat absorbed	BTU/HR
CAL DUT	Calculated duty	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

Controller: SET/VARY-UNTIL Variables for Flash

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
HEA	Heat addition	BTU/HR
LIQ FRA	Specified liquid fraction	*
PRE OUT	Pressure	PSIA
TEM OUT	Temperature	R

* mole fraction stored as (+), mass fraction stored as (-)

Controller: SET/VARY-UNTIL Variables for Flowmeter

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Heat Exchanger

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
TEM OUT	Temperature out for 1st inlet stream	R
TEM APP	2nd inlet temperature - 1st outlet temperature	R
DEL TEM	1st outlet temperature - 1st inlet temperature	R
DUT	Duty	BTU/HR
ARE	Area	FT2
PRE REF	Pressure of refrigerant stream	PSIA
TEM REF	Temperature of refrigerant stream	R
TEM WAT IN	Temperature cooling water in	R
TEM WAT OUT	Temperature cooling water out	R
DEL (i)	Pressure drop shell (1), tube (2)	PSI
CAL ARE	Calculated area	FT2
CAL LMT	Calculated log mean temperature difference	
CAL DUT	Calculated duty	BTU/HR
CAL WAT	Calculated cooling water for single stream exchanger	GAL/HR
CAL EFF ARE	Calculated effective area	FT2
CAL ACT ARE	Calculated actual area per defined geometry	FT2
TEM AIR IN	Temperature of air inlet	R
TEM AIR OUT	Temperature of air outlet	R
CAL AIR	Calculated air flowrate	LBMOL/HR

Controller: SET/VARY-UNTIL Variables for Hydrotreater Reactor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Line

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
INS DIA	Inside diameter	FT
nominal DIA	Nominal diameter	FT

Controller: SET/VARY-UNTIL Variables for LNG Exchanger

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
----------------	-----------------------	-------

ARE (i)	Area per shell	FT2
CAL ARE (i)	Calculated area for tube i	FT2
CAL DUT (i)	Calculated tubeside duty	BTU/HR
CAL LMT (i)	Calculated LMTD (i)	R
CAL MIX TEM	Temperature shell feed after tubeside recycle	R
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
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.

Controller: SET/VARY-UNTIL Variables for Mixer

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Multiple Flash

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Multiple Phase Flash

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Phase Envelope

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Phase Map

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Plate-Fin Exchanger

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

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Module/Keyword	Parameter Description	Units
TEMPerature APProach HOT side	Temperature approach on hot side	R
TEMPerature APProach COLD side	Temperature approach of cold stream	R

Controller: SET/VARY-UNTIL Variables for Plug Flow Reactor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Polytropic Compressor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
CAL SPE	Calculated Speed	RPM
CAL SUC VOL	Calculated suction volume	FT3/MIN
PRE OUT	Outlet pressure	PSIA
SPE	Radial speed	RPM
THE FAC	Thermodynamic factor	----

Controller: SET/VARY-UNTIL Variables for Pump

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
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.

Controller: SET/VARY-UNTIL Variables for Reactor

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
CON	Conversion of the limiting reactant	----
TEM OUT	Temperature out R	R
HEA	Heat of reaction BTU/HR	BTU/HR
DEL	Delta pressure PSIA	PSIA
DUT	Specified Duty BTU/HR	BTU/HR
CAL DUT	Calculated reactor duty BTU/HR	BTU/HR
TEM APP COSHIF	Temperature Approach of CO Shift	R
TEM APP METHAN	Temperature Approach of Methanation	R
TEM APP MET SYN	Temperature Approach of Methanol Synthesis	R
TEM APP AMM SYN	Temperature Approach of Ammonia Synthesis	R

Controller: SET/VARY-UNTIL Variables for Refine Distillation Column

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
NONE	There are no specifications and this module is not available for use with Controller.	n/a

Controller: SET/VARY-UNTIL Variables for Shortcut Fractionator

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
CAL DUT CON	Calculated condenser duty	BTU/HR
CAL DUT REB	Calculated reboiler duty	BTU/HR
CAL FEE TRA	Calculated feed tray	----
CAL MIN REF	Calculated minimum reflux ratio (RR)	----
CAL MIN STA	Calculated minimum number of stages	----
CAL REF	(PER MIN) (CAL MIN REF)	----
CAL STA	Number stages at specified RR	----
DEL	Column pressure drop	----
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	----

Controller: SET/VARY-UNTIL Variables for Stream Manipulator

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
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.	BTU/LBMOL
CAL SCF	Calculated value per SCF of input stream. The description of the VALUE/SCF calculated value is the same as for CAL MOL.	BTU/SCF
FAC (i)	Factor by which "ith" component is to be ADDED SUBtracted, MULTIplied or DIVided.	----

Controller: SET/VARY-UNTIL Variables for Stream Properties

A complete list of stream parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
ENTH	Total stream enthalpy	BTU/HR
ENTR	Total stream entropy	BTU/HR/R
FLO	Molar Flowrate of Stream	LBMOL/HR
FLO MAS	Mass Flowrate of Stream	LB/HR
FLO COM i	Molar Flowrate of component ID#	LBMOL/HR
FLO COM MAS i	Mass Flowrate of component ID#	LB/HR
FLO MAS COM i	Mass Flowrate of component ID#	LB/HR
FLO COM FRA i	Flowrate fraction of component ID#	---
PRE	Stream Pressure	PSIA
TEM	Stream Temperature	R
VAP FRA	Molar Vapor Fraction	----
VAP MASS FRA	Mass Vapor Fraction	----
REI VAP PRE	Reid vapor pressure	PSI

Controller: SET/VARY-UNTIL Variables for Tank

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
<u>Tank</u>		
PRO FLO i	Product FLOWrate of "ith" stream	LBMOL/HR

Controller: SET/VARY-UNTIL Variables for Valve

A complete list of equipment parameters which can be accessed by SET and VARY-UNTIL controller commands are shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

Module/Keyword	Parameter Description	Units
----------------	-----------------------	-------

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DEL
PRE OUT
TEM BUB
TEM DEW

Pressure drop across valve
Outlet pressure
Temperature for specified PRE OUT at BUB PT
Temperature for specified PRE OUT at DEW PT

PSI
PSIA
R
R

Controller Examples

There are several sample flowsheets in “Chapter 14: Controller Samples - c:\designii\samples\equipmnt\cont” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 9: Continuous Stirred Tank Reactor

This reactor model assumes a steady state flow of species for the reactor and that the concentrations of species and temperature are uniform throughout the reactor. It uses a Quasi-Newton method to solve a series of equations which determine the outlet compositions for the reactor. Multiple reactions can be specified for the CSTR. Mass and energy balance calculations assume perfect mixing conditions. In addition, you can employ the default power law kinetics model or user specified models for particular reactions.

CSTR Types

There are four CSTR types that you can model using DESIGN II:

- Isothermal
- Temperature out
- Adiabatic and
- Adiabatic with a specified duty

All the important parameters, such as reaction expressions, calculated duty, reactor type, and other related specifications will be reported in the Equipment Summary section of your output. The compositions, temperature, and pressure of the CSTR product will be reported in the Stream Summary and Detailed Stream sections.

CSTR Command Details

CSTR Major Specifications

(enter the following required command)

VOLume (L3 units) =

Enter the volume of the reactor.

CSTR Reactor Type Specification

(Choose only one of the following 3 options)

ISOthermal

Enter isothermal reactor keyword command. For CSTR this is the default reactor type. Product stream enthalpy is calculated using the feed stream temperature.

TEMperature **OUT** (T units) =

Enter the required outlet temperature for a CSTR

ADIabatic

Product stream enthalpy is equal to the feed stream enthalpy plus the heat of reaction, and the temperature of reactor product is calculated. Allows an optional heat duty specification.

CSTR Adiabatic Reactor Commands

(Choose any of the following commands)

HEAt added (H units/t units) =

Enter an optional heat duty specification.

TEMperature **OUT** **GUE**ss (T units) =

Enter an initial guess for the outlet temperature for an ADIabatic (or ADIabatic, HEAt added) reactor type.

CSTR Reaction Stoichiometry Commands

R i = (**a1*****r1** + **a2*****r2** + = **b1*****p1** + **b2*****p2** +...)

Enter a reaction command for each reaction.

i

a1,a2

r1,r2

b1,b2

p1,p2

is the reaction number

are stoichiometric coefficients for the reactants

are component ID numbers for the reactants

are stoichiometric coefficients for the products

are component ID numbers for the products.

CSTR Reaction Kinetics Commands

All of the following commands are required, regardless of the reactor type you have chosen. These three items, which determine the rate of the reaction, can also be defined using Inline FORTRAN. This allows you to override the power law model by specifying the kinetics directly.

ORDER of reaction $i = r1, Or1, r2, Or2$

Enter the partial order of each reactant

i	is the reaction number,
$r1, r2$	are component ID numbers for the reactants
$Or1, Or2$	are partial orders for the corresponding reactant.

FREquency factor (L3 units, molar Q units, t units) = $i1, fi1, i2, fi2$.

Enter the frequency factor (ko)

$i1, i2$	are the reaction numbers
$fi1, fi2$	are frequency factors for corresponding reaction.

ACTivation energy (H units/molar Q units) = $i1, Ei1, i2, Ei2$

Enter the activation energy (Eo)

$i1, i2$	are reaction numbers
$Ei1, Ei2$	are activation energies for the corresponding reaction.

NOTE: The order of the dimensional units for the FREquency factor command cannot be changed. The program will automatically determine whether volume or area units are appropriate from the ORDER command.

RATE $i = f(\text{CONC } j, \text{TEM}, \text{PRE})$

The **FRE**, **ORD**, and **ACT** commands can be replaced with an Inline FORTRAN expression where:

i	is the reaction number,
RATE	is a required inline FORTRAN keyword,
CONC	is a keyword representing concentration,
j	is the component ID number,
TEM	is a keyword for temperature within the reactor,
PRE	is a keyword for pressure within the reactor.

CSTR Example Using Inline Fortran To Replace Fre, Ord, And Act Commands

Reaction

$C2H4 + H2 \rightarrow C2H6$ $ko = 5.0457E13 \text{ FT}^2/\text{LBMOL-HR}$ $Eo = 5.8845E4 \text{ BTU/LBMOL}$

The rate of this reaction can be expressed as

frequency $e^{Eo/(R*TEM)}$ * $CONC2^2 * CONC1^x$

where:

R is the gas constant, y is the power term for ethylene, x is the power term for hydrogen.

Using Inline FORTRAN, the reaction rate is defined as

```
R2=(1*22 + 1*1 = 1*3)
F- DURING
F- RATE2 = 5.0457E13*EXP(-.58845E4/(R*TEM)) *CONC22*CONC1
```

CSTR Required Commands For Components With Id Numbers >> 98

The CSTR calculation requires heat of formation data. The DESIGN II data base contains heat of formation data for components with ID numbers from 1 through 98. If you specify a component with an ID greater than 98, you must supply its corresponding heat of formation data. Enter heat of formation data at 25 C with one of the following commands depending on the feed phase. The selected command must appear in the GENERAL section.

HEAT of **FOR**mation (H units/molar Q units) $i =$ or

Enter the heat of formation for component i , where i is the component ID number. Used when the data is on a vapor basis.

HEAT of **FOR**mation of **LI**quid (H units/molar Q units) $i =$

Enter the heat of formation for component i , where i is the component ID number. Used when the data is on a liquid basis.

For example,

```
GENeral
  components = 2,49,48,62,1021
  HEAT of FORMation (BTU/LBMOL) 1021 = -86544
```

CSTR Command Summary

Major Specifications

VOLume (L3 units) =

Reactor Type Specification

ISOthermal

TEMperature **OUT** (T units) =

ADiabatic

Adiabatic Reactor Commands

HEAt added (H units/t units) =

TEMperature **OUT** guess (T units)

Additional Component Specification Commands

HEAt of **FOR**mation (H units/molar Q units) **i** =

HEAt of **FOR**mation of **LIQ**uid (H/molar Q units) **i** =

ENTropy of **FOR**mation (H/molar Q units/T units) **i** =

Reaction Kinetics Commands

ORder of reaction **i** = r_1, Or_1, r_2, Or_2

FREquency factor (L units, molar Q units, t units)
= $i_1, f_{i1}, i_2, f_{i2} \dots$

ACTivation energy (H units/molar Q units)
= $i_1, E_{i1}, i_2, E_{i2} \dots$

RATe **i** = $f(\text{CONC } j, \text{TEM}, \text{PRE})$

Reaction Stoichiometry Commands

R i = $(a_1 * r_1 + a_2 * r_2 + \dots = b_1 * p_1 + b_2 * p_2 + \dots)$

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

CSTR Optional Command: Lost Work Analysis

If a lost work analysis is specified with the **LOSt WORK** command in the **GEN**eral section, the **ENT**ropy of formation data also must be entered in the **GEN**eral section with the following command.

ENTropy of **FOR**mation (H units/molar Q units/T units) **i** =

Enter the entropy of formation for component **i**, where **i** is the component ID number. The allowable units are:

BTU/LBMOL/R (default)

CAL/GMOL/K

KJ/KGMOL/K

J/GMOL/K

KCAL/KGMOL/K

CSTR Step by Step

CSTR STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

CSTR

Assigned equipment flowsheet number

User choice - up to 16 characters

One only

One only

CSTR STEP 2

Specify the volume of the reactor. Reactor volume specification.

Volume

VOL (L3 units) =

CSTR STEP 3

Choose one of the three reactor types listed below. Isothermal reactor (enter the following command)

Isothermal reactor (default)

ISO

Temperature out reactor (enter the following command)

Temperature out specification

TEM OUT(T units)=

Adiabatic reactor (enter the following commands)

Adiabatic reactor keyword command

Optional heat duty specification

Optional product temperature guess

ADI

HEA (H units/t units) =

TEM OUT (T units) =

CSTR STEP 4

Enter the information required listed below to define reaction stoichiometry. Reaction stoichiometry specification.

Reaction stoichiometry for each reaction

Ri = $(a_1 * r_1 + a_2 * r_2 + \dots = b_1 * p_1 + b_2 * p_2 + \dots)$

- **i** reaction number,
- **a1,a2** stoichiometric coefficients for the reactants
- **r1,r2** component ID numbers for the reactants

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- b1,b2 stoichiometric coefficients for the products
- p1,p2 component ID numbers for the products

CSTR STEP 5

Enter the information listed below to define the reaction kinetics or use Inline FORTRAN to define reaction kinetics.
Partial order of each reactant.

Order of reaction **ORD i = r1, Or1, r2, Or2**

- i reaction number,
- r1,r2 component ID numbers for the reactants
- Or1,Or2 partial orders for the corresponding reactant

Frequency factor (ko) and activation energy (Eo) specification

Frequency factor (order of the dimensional units for the **FRE** (L3 units, molar Q units, t units) = i1, fi1, i2, fi2 ..
FREquency factor command cannot be changed)

- i1, i2 reaction numbers
- fi1, fi2 frequency factors for the corresponding reaction

Activation energy **ACT** (H units/molar Q units) = i1, Ei1, i2, Ei2 ..

- i1, i2 reaction numbers
- Ei1, Ei2 activation energies for the corresponding reaction

Inline FORTRAN reaction kinetics command

Rate (see reference section for additional information) **RAT i = f(CONCj, TEM, PRE)**

- i reaction number
- RAT required inline FORTRAN keyword
- CONC keyword representing concentration
- j component ID number
- TEM keyword for temperature within the reactor
- PRE keyword for pressure within the reactor

CSTR STEP 6

For components with ID numbers greater than 98, enter the heat of formation data.

Enter ONE of the following heat of formation commands based on the reactor feed phase.

Heat of formation of component "i", where "i" is the component ID number. **HEA FOR** (H units/molar Q units) i =
Used if data is on a vapor basis; (place command in the GENeral section)

Heat of formation of component "i", where "i" is the component ID number. **HEA FOR LIQ** (H units/molar Q units) i =
Used if data is on a liquid basis; (place command in the GENeral section)

Choose any of the optional commands listed below:

If LOST work command is entered in GENeral section, THEN enter the following:

NOTE: LOST work analysis requires both heat of formation and entropy of formation data for all components. For components 98 this data is available in the pure component database. For components with ID number > 98 enter this data with the HEA FOR command in step 6 and the ENT FOR command above.

Entropy of formation where "i" is the component ID number. (place **ENT FOR** (H units/molar Q units/T units) i =
command in the GENeral section)

IF thermo is different from global (GENeral section) options THEN select:

- K-value option **KKE =**
- Enthalpy option **HKE =**
- Density option **DKE =**

CSTR Examples

There is a sample flowsheet in "Chapter 15: Continuous Stirred Tank Reactor (CSTR) Samples - c:\designii\samples\equipmnt\cstr" of the DESIGN II for Windows Tutorial and Samples Guide.

CSTR References

1. Smith, J.M., *Chemical Engineering Kinetics*, 3rd Ed., New York, 1981.
2. Froment, Gilbert F., and Bischoff, Kenneth B., *Chemical Reactor Analysis and Design*, John Wiley & Sons, New York, 1979.

Chapter 10: Depressuring

Depressuring systems are used extensively in process plants for protecting vessels from overpressure. Overpressuring has many causes, such as external fire, exothermic reactions, loss of power, inadequate cooling, and blocked lines. Depressuring systems are needed to prevent equipment from rupturing and to provide safety for plant personnel. API RP-521 recommends that vessel pressure should be reduced to 100 PSIG or 50% of design pressure, whichever is lower, in fifteen minutes.

Both pure components and mixed phase venting are allowed in addition to vapor phase venting.

Depressuring Analysis Methodology

The depressuring analysis is based on a vessel which is exposed to an external fire. The program calculates the pressure buildup in the closed vessel until the pressure reaches the set pressure of the valve. The conditions during the blowdown period after the opening of the depressuring valve are also calculated. The blowdown period is divided into several intervals with important variables reported for each time interval.

One inlet and one or two outlet streams may be coded. The second outlet stream is used with PRInt options 2 or 3. This will print stream properties for the vent gas stream at the time of maximum flowrate. The temperature, pressure and composition of the inlet stream are assumed to be the operating conditions of the vessel. A flash is performed to determine the vapor and liquid compositions and initial flow rates. The DEPressuring module will yield more meaningful results if heat as a function of wetted surface area is used. This option includes commands describing the vessel diameter, the vessel orientation, vessel length, and the liquid height.

Several assumptions are made for the depressuring analysis:

1. Flow to vessel is stopped (i.e. no fresh feed).
2. The heat involved is provided externally either at a constant rate ($\Delta Q = \text{Const. BTU} / \text{Time}$) or as a function of the wetted surface area ($\Delta Q = 21000 * F A_w^{0.82}$) where F is an environmental factor recommended by API RP-520 and A_w is wetted surface area. The wetted surface area factor can be varied to 21000 - only if facilities are equipped with fire fighting equipment and adequate drainage.
3. The vent flow (vapor or mixed) through the valve is either a choking flow or subsonic flow due to sufficiently large back pressure.
4. If the vessel contents are all vapor then the heating of the fluid due to the external heat source will be obtained by calculating the heat added assuming that the tank was full of liquid and then scaling the wetted wall heating factor by the ratio of the vapor density to the liquid density.
5. The temperature of the vessel contents equals the temperature of the feed stream.
6. The pressure of the vessel contents equals the pressure of the feed stream.
7. The composition of the vessel contents equals the composition of the feed stream.
8. If the contents of the vessel are all liquid and the venting is set to vapor, the vessel will vent liquid until vapor is available to vent.
9. If the feed stream is all vapor then the user specified initial liquid height will be ignored and set to zero.
10. If the feed stream is all liquid then the user specified initial liquid height will be used.
11. If the feed stream is mixed phase then the user specified initial liquid height will be ignored and the liquid height will be set to the equilibrium liquid height between the vapor and liquid phases.

Methods used from API 520 Edition 7.

1. All vapor venting for critical and sub critical regimes are included (section 3.6.2 and 3.6.3). Includes corrections for combined rupture disk/valve and only rupture disk options. Correction for balanced bellows valve is available.
2. Steam relief at critical flow (vapor venting option). Also includes rupture disk combinations.
3. Liquid relief for valves not requiring capacity certification. Also includes rupture disk combinations.
4. Two phase (liquid/vapor) relief using Appendix D. of API code. This includes options 1 and 3, critical and sub-critical conditions. Rupture disk combinations are included.
5. Subcooled liquid relief with flashing in orifices and with a non-condensable gas. Rupture disk combinations are included along with corrections for balanced bellows valve. Overpressure correction (Fig D-2) not included.

Depressuring Analysis Command Details

Depressuring Relief Valve Description

CROss Sectional Area Of Valve (L Units) =

Enter the cross-sectional area for the valve.

COEfficient of discharge =

Enter manufacturer's specification. Default is 1.0.

Depressuring Geometry and Initial Contents

Following are commands to input heat as a function of wetted surface area. To give heat at a constant rate, use *Depressuring*

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Heat Transfer To Vessel Commands instead of Geometry and Initial Contents Commands.

DIA (L units) =

Enter the diameter of the vessel to use for predicting heat transfer based on wetted surface area.

HORizontal

VERtical

SPHerical

Enter one of the vessel configurations for calculation of wetted surface area. Default is VERTICAL.

The composition of the vessel contents is determined from the inlet stream. If any of the necessary dimension specifications are not entered, the vessel size will be calculated assuming a one hour residence time. If the depressuring analysis will be calculated with heat as a function of wetted surface area, you can enter the commands below which will adjust the rate of the vapor and liquid portions of the streams (using inlet compositions).

LENGth (L units) =

Enter the length of the vessel for horizontal or vertical vessel configuration.

Initial **LIQ**uid **HEI**ght (L units) =

Enter the initial height of the liquid from the bottom of the vessel.

RUPture Disk Factor =

Enter rupture disk factor (OR) one of the following rupture disk factor options to be used in the relief valve.

Default is 1.

0 < factor < 1 = value of factor between 0 and 1 to be used by program.

0 or 1 = no rupture disk

2 = rupture disk and relief valve present (factor used is 0.9)

3 = only rupture disk (factor used is 0.62).

BALanced Bellows Factor =

Enter the back pressure correction factor (or) one of the following back pressure correction factor options to be used for balanced-bellows pressure relief valve. This factor is used only when the relief valve is used for liquid venting only. A balanced pressure relief valve is used where the built-up back pressure is high (or) where the super-imposed back pressure varies widely compared to set pressure. Default is 1.

0 < factor < 1 = value of factor between 0 and 1 to be used by program.

2 = balanced bellow factor calculated by figure 3 in API 520, 7th edition.

BACK Pressure **FACTOR** =

This back pressure factor is used when balanced-bellows pressure relief valves are used in vapor venting. Default is 1.

Depressuring Heat Transfer to Vessel Commands

Following are commands to input heat at a constant rate. To give heat as a function of wetted surface area, use *Depressuring Geometry and Initial Contents* commands instead of Heat Transfer to Vessel Commands.

You have two choices for entering the heat involved in the depressuring analysis: heat added at a constant rate or heat as a function of wetted surface area. Default is heat transfer based on wetted surface area.

HEAt absorbed (H units) =

Enter the constant rate of external heat which will be applied to the vessel. For depressuring without heat enter HEAt = 0 and specify a set pressure that is lower than the vessel operating pressure.

WETted surface area factor =

Enter the wetted surface area factor. Default is 34500 .

Depressuring Analysis Optional Command Details

Depressuring Pressure Specifications

REDuced pressure (P units) =

Enter the reduced pressure. Default is 100 PSIA or 50% of operating pressure, whichever is lower.

BACK pressure (P units) =

Enter a value if a subsonic flow condition is desired (non-choking flowrate). If the back pressure is higher than critical-flow pressure, the resulting vapor flowrate will be lower. Default is 14.696 PSIA.

SET pressure (P units) =

Enter the pressure at which the valve is to open. Default for set pressure is 10% above operating pressure.

Depressuring Environment Specification

ENVironmental factor =

Enter an environmental factor for type of installation. Default is 1. See table below for typical values.

Type of Installation

Factor F

1. Bare vessel

1.0

2. Insulated vessels (arbitrary insulation conductance values are shown as examples and are in BTU/HR/FT2	
a. 4.0	0.3
b. 2.0	0.15
c. 1.0	0.075
3. Water-application facilities, on bare vessel	1.0
4. Depressuring and emptying facilities	1.0
5. Underground storage	0.0
6. Earth-covered storage, above grade	0.03

Depressuring Calculation Option

VENT MIXed

Use this command to specify that the mixed contents of a container are vented. Default is vapor venting, if the vapor volume fraction is greater than 10%.

Examples:

1. Saturated liquid/vapor propane system enters relief valve and both phases are vented.
2. Highly subcooled propane and nitrogen enters relief valve and both phases are vented.
3. Subcooled propane enters relief valve and is vented.
4. Saturated (or subcooled) liquid/vapor propane system and nitrogen enters relief valve and both phases are vented.

TIME STEp (t units) =

Use this command to specify the time intervals for the depressuring calculations. The default interval is one minute. Note that the default time unit is hours.

MIN TIME (t units) =

Use this command to specify the minimum time required for depressurizer to complete its specified calculations. The default minimum time is 15 minutes per EPA (Environmental Protection Agency in USA).

OPEN TIME (t units) =

Use this command to open the valve linearly over time when the depressurizer readies itself to open. With this optional specification the valve opens linearly over the specified time period. The amount of flowrate through the valve will be severely cut for a specified time period before it opens to use full throat area. Without this optional command, the valve will open to use 100% throat area immediately. The default is zero.

NOTE: The percentage valve opening is only printed in depressurizer module results when the optional PRINT = 3 is used.

MAX TIME (t units) =

Use this command to specify the maximum time required for depressurizer to complete its specified calculations. The default maximum time is 60 minutes. Note that this time applies for both pressurization and venting processes of the module.

Valve RESeat pressure (P units) =

Use this command to specify the valve reseal pressure during its specified calculations. At this reseal pressure (chosen by user to be below the set pressure but above the back pressure), there will be no relief flow until the pressure again reaches the set pressure to continue relieving. The default is zero psia.

VAPor (fraction) =

Use this command to specify an optional minimum vapor volume fraction of the tank to be vented as vapor only instead of mixed phase. The default is 10 % by volume.

Depressuring Print Options

PRInt = 1

Same as the default print option except that the DEPressuring analysis table flow rates are reported in mass units rather than molar units.

PRInt = 2

Reports the vent gas temperature as well as the information reported in PRInt = 1.

PRInt = 3

Uses same format as stream summary. The vent gas flow rate for each component is reported as well as the enthalpy and heating rate for each interval.

The DEPressuring module will also print stream properties for the vent gas stream at the time of maximum flowrate (i.e. when the depressuring valve first opens). This provides the user with the required information to size the depressuring line, if desired. This option is available when the PRInt options 2 or 3 are used. To activate this feature, just add a second outlet stream number to the DEPressuring module. For example:

```
DEPressuring 1 = V101, 1, -2, -3
```

Depressuring Command Summary

Relief Valve Specification

CROss sectional area of valve (L units) =
COEfficient of discharge =

Geometry and Initial Contents

DIA (I UNITS) =
 and
HORizontal
VERtical
SPHerical
LENgth (I units) =
LIQuid **HEI**ght (L units) =
RUPture Disk Factor =
BALanced Bellows Factor =
BACK Pressure **FAC**tor =

Pressure Specifications

REDuced pressure (P units) =
BACK pressure (P units) =
SET pressure (P units) =

Heat Transfer to Vessel Commands

HEAT absorbed (H units) =
WETted surface area factor =

Print Options

PRInt = 1, 2, or 3

Calculation Option

VENT MIXed
TIME STEP (t units) =
OPEN TIME (t units) =
MAX TIME (t units) =
REseat pressure (P units) =
VAPor (fraction) =

Environment Specification

ENVironmental factor =

Thermodynamic Commands

HKEy=
KKEy=
DKEy=

Depressuring Step by Step

Depressuring STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
 Equipment number
 Equipment name
 Inlet stream
 Outlet streams

DEP
 Assigned equipment flowsheet number
 User choice - up to 16 characters
 One only
 One or two

The 2nd outlet stream is used with PRInt options 2 or 3 to print stream properties for the vent gas stream at the time of maximum flowrate (i.e., when the depressuring valve first opens).

Depressuring STEP 2

Enter relief valve data.

Cross-sectional area of the valve
 Optionally, coefficient of discharge

CRO (L units) =
COE =

Depressuring STEP 3

Define geometry and initial contents of vessel (Enter ALL of the following)

Vessel diameter
 Vessel orientation (choose ONE)
 - Horizontal
 - Vertical
 - Spherical
 Initial vessel contents (enter both)
 - Vessel length
 - Liquid height

DIA (L units) =

HOR
VER
SPH

Rupture disk factor (OR) one of the following rupture disk factor options to be used in the relief valve. Default is 1.
 0 < factor < 1 = value of factor between 0 and 1 to be used by program.
 0 or 1 = no rupture disk
 2 = rupture disk and relief valve present (factor used is 0.9)
 3 = only rupture disk (factor used is 0.62).

LEN (L units) =
LIQ HEI (L units) =
RUPture Disk Factor =

Back pressure correction factor (or) one of the following back pressure correction factor ptions to be used for balanced-bellows pressure relief valve. Used for **liquid venting** only. Default is 1.
 0 < factor < 1 = value of factor between 0 and 1 to be used by program.
 2 = balanced bellow factor calculated by figure 3 in API 520, 7th edition.
 This back pressure factor is used when balanced-bellows pressure relief valves are used in **vapor venting**. Default is 1.

BALanced Bellows Factor =

BACK Pressure **FACTOR** =

Depressuring STEP 4

Choose a method of heat transfer to the vessel (enter ONE of the following)

Heat added as a function of wetted surface area (default)
 Heat added at a constant rate
 Wetted surface area factor

HEA (H units/t units) =
WET =

OPTIONAL - Choose any of the optional specifications listed below:

Pressure specifications

Final vessel pressure after blowdown
 Back pressure downstream
 Set pressure

RED (P units) =
BAC (P units) =
SET (P units) =

Installation type

Environmental factor

ENV =

Calculation option

Specify that the mixed contents of a container are Vented. Default is vapor venting, if the vapor volume fraction is greater than 10%.
 Time interval for the depressuring calculations (default is 1 min; default time unit is hours)
 Use this command to open the valve linearly over time (default is zero). Results when on **PRI =3** only.
 Use this command to specify the maximum time required for depressurizer to complete its specified calculations. The default maximum time is 60 minutes.
 Use this command to specify the valve reseal pressure during its specified calculations. The default is zero psia.
 Use this command to specify an optional minimum vapor volume fraction of the tank to be vented as vapor only instead of mixed phase. The default is 10 % by volume.

VENT MIXed

TIM STE (t units) =

OPEN TIME (t units) =

MAX TIME (t units) =

RESeal pressure (P units) =

VAPor (fraction) =

Print options (choose ONE)

Flow rates reported in weight/time units rather than mole/time units
 Similar to above, plus vent gas temperature
 Same as above plus added heat, enthalpy and downstream pressure
 IF thermo is different from global (GENeral section) options THEN select
 K-value option
 Enthalpy option
 Density option

PRI = 1
PRI = 2
PRI = 3

KKE =
HKE =
DKE =

Depressuring Analysis Examples

There are several sample flowsheets in "Chapter 16: Depressuring Samples - c:\designii\samples\equipmnt\depres" of the DESIGN II for Windows Tutorial and Samples Guide.

Depressuring Analysis References

1. API Recommended Practice 520, "Recommended Practice for the Design and Installation of Pressure-Relieving Systems in Refineries, Part I-Design", 7th Ed., American Petroleum Institute, Washington, D.C., Jan 2000.
2. API Recommended Practice 521, "Guide For Pressure Relief and Depressuring Systems", 1st Ed., American Petroleum Institute, Washington, D.C., 1969.

Chapter 11: Distillation Column

The DISTillation column module is used for rigorous simulation of absorbers, fractionators, strippers and other types of single-column configurations. Most single-column units can be modeled, including demethanizers, stabilizers, sour water strippers, amine contactors and regenerators, and azeotropic distillation towers. This module can be used for design, modification, or optimization of rigorous distillation columns. Extensive thermodynamic options are available (see *Thermodynamics Section*). With the use of the proper option, the operation of existing units can be duplicated within several percent of actual plant data.

Distillation Features

Column Types

The DISTillation module offers a great deal of flexibility in the definition of column configurations. Six major column types are available distinguished by the presence or absence of condensers or reboilers. Additionally, an essentially unlimited number of feeds, feed components, products, trays, and heaters/coolers are allowed.

Product Specification And Column Control

The flexibility of the DISTillation module also includes the control of the fractionation process. Component purities, recoveries, or ratios can be specified directly in top, bottom, or side products. Product rates can be set in mass, molar, or volumetric units. Reboiler or condenser temperatures and duties can be specified as can reflux ratio or reflux flowrate. Additional specifications can be created with *Inline FORTRAN*.

Calculation Techniques

Four methods are available for solving the rigorous tray-to-tray heat and material balances for your column. These are [Regular](#), [SUPER](#), [SUPER PLUs](#), and [SUM RATES](#). The trays, partial condensers, and reboilers are modeled as equilibrium stages. Special commands allow the convergence algorithms to be fine tuned to meet user specified tolerances.

Water K-values And Decant

The K-value option you choose for your simulation normally determines whether water (if present) is treated miscibly or immiscibly in the column (see *Thermodynamics: Water K-Values in Hydrocarbon Systems* for details). *Free* water is not decanted automatically. If you specify a water decant from the condenser or any tray(s), the amount of *free* water formed at the temperature and pressure of the condenser or tray is calculated automatically. You may also specify the solubility of water in the reflux returning to the column. The default solubility will be based on the water-in-kerosene chart from the API Technical Data Book. You can enter an estimate for the fraction of free water in the liquid on the trays. You can request a check for free water on trays where no decants have been established.

Stream Order Convention

Certain conventions must be followed when defining feed and product streams in the DISTillation module. These conventions are listed below:

- Each feed stream to the DISTillation module is assigned a unique number. The feed stream numbers are listed in top-to-bottom order.
- Each product stream is assigned a unique number. The product stream numbers are given negative signs and listed in top-to-bottom order.
- Decant streams from the condenser or any tray are not counted as a product and do not require a stream number.
- Internal streams, such as reboiler or reflux streams, except when the streams are used in conjunction with an internal stream command are not numbered. Their compositions, flowrates, and other properties are reported automatically in the column results.

Tray Numbering Convention

Certain conventions must be followed when numbering trays in the DISTillation module. Tray numbers are used to locate feeds, side draws, side heater/coolers, and intercoolers.

- All trays are theoretical trays.
- Trays are numbered from top-to-bottom. The top tray is always tray one. The number of trays entered does not include a condenser or a reboiler. If present, the program handles them automatically numbering the condenser tray zero and the reboiler one larger than the number of trays.

Step-by-Step Procedure

Specifying a rigorous DISTillation column with DESIGN II is simple when following. The procedure is summarized below:

- Define the column type by selecting the combination of condenser and/or reboiler.
- Add required column configuration commands
- Determine the number of heat and material balance specifications required based on the column type and select the one(s) for your simulation.
- Add any side draws, heaters/coolers, intercoolers, and water decant commands.
- Add optional commands as needed for additional calculations such as reboiler or condenser curves CO2 freeze prediction, extra plots, column sizing, internal stream reports and others.

Distillation Command Details

Distillation: Column Type

Eight column types are available in the DISTillation module. The correct column type selection is based on whether the column has a condenser and/or a reboiler. Once the column type is selected, an essentially unlimited number of feeds, products, trays, side heater/coolers, and intercoolers can be added. Select the appropriate column type below:

ABSORber

Any column with no condenser and no reboiler. A liquid feed to the top tray and a vapor feed below the bottom tray are required. An optional PRESATurator may be added.

ABSORber with REBoiler

Any column with no condenser but with a reboiler. A liquid feed to the top tray is required. An optional PRESATurator may be added.

PRESATurator and TEMperature of CHiller (T units) =

The PRESATurator configuration can only be added to the ABSorber and ABSorber with REBoiler column types. If used, the TEMperature of CHiller command must also be entered. The top feed location is specified as tray zero. Regular convergence technique only.

LLE

Any column with no condenser and no reboiler. Liquid feed to the top tray and liquid feed to the bottom tray.

STRipper

Any column with a partial condenser but no reboiler. A vapor feed below the bottom tray is required.

STRipper with TOTal condenser

Any column with a total condenser but with no reboiler. A vapor feed below the bottom tray is required.

PARTial fractionator

Any column with a partial condenser and a reboiler. A minimum of one feed and two products is required.

TOTal fractionator

Any column with a total condenser and a reboiler. A minimum of one feed and two products are required.

Distillation: Required Column Description

All the commands in this section are required for all column types. The commands provide the following basic column description:

- Number of theoretical trays
- Temperature guesses for the top and bottom products
- Pressure of the column
- Feed tray locations
- Molar product flowrates

Number Of Theoretical Trays**TRays =**

Enter the number of theoretical trays in the column (not including the condenser and reboiler if present).

The top tray is always tray 1. The trays are numbered from top-to-bottom. Do not count the condenser or reboiler in the number of trays. The program numbers the condenser as tray zero and the reboiler as one greater than the number of trays. A minimum of two theoretical trays are allowed.

Column Temperatures**TEMperature TOP guess (T units) =**

Enter the top product temperature as an initial guess. If the TEMperature of CONDenser command is also entered, then TEMperature TOP is the top tray temperature.

TEMperature BOTtom guess (T units) =

Enter the bottom product temperature as an initial guess.

A linear initial column profile is estimated from these temperature guesses for most columns (except a quadratic profile is used for the reboiled absorbers). In some cases, where the temperature profile is far from linear, it may be better to estimate the top or bottom temperature different from the actual temperature. Specifically, addition (or removal) of heat to tray(s) with an intercooler or side heater/cooler can cause a nonlinear temperature profile. In cases where nonlinear column temperature profiles are expected, a temperature profile for every tray in the column can be entered and may be required for convergence (see *Distillation: Column Profiles* for details).

To estimate the product temperatures consider running a SHORtcut column or a COMponent SPLitter. Both modules provide guesses for the product rates as well as the top and bottom temperatures.

Column Pressures**PREssure of TOP tray (P units) =**

Enter the top tray pressure. If the optional PREssure of CONDenser is not entered (see *Distillation: Condenser Commands*), the top tray pressure will be used as the pressure of the top product. If a nonlinear pressure profile is suspected or known to exist, the complete PREssure PROfile, pressure of every tray, can be entered (see *Distillation: Column Profiles* for details).

PREssure of BOTtom tray (P units) =

Enter the bottom tray pressure. If the optional PREssure of REBoiler is not entered (see *Distillation: Pressure Profile*), the bottom tray pressure will be used as the pressure of the bottom product. If a nonlinear pressure profile is suspected or known to exist, the complete PREssure PROfile, pressure of every tray, can be entered (see *Rigorous Distillation Column Profiles* for details).

DELta pressure (P units) =

Enter the pressure drop from the bottom product pressure to the top tray pressure. Specifying pressure drop will override PREssure of BOTtom tray. Default is zero.

Feed Tray Location

Feeds can enter on any theoretical tray in the column. The top tray is always tray one and the condenser, if present, is tray zero. The feed tray location is the tray where any liquid in the feed would go. This means if the feed is two phase at the tray pressure, then the liquid portion of the feed enters the feed tray and the vapor portion automatically mixes with the tray above. Likewise if the feed is all vapor, then the vapor enters and mixes with the liquid in tray above the feed tray.

Feeds are always adiabatically flashed at the tray pressure. If the feed pressure is less than the tray pressure, calculations will continue but a warning message will state that a feed pump is required.

LOCation of FEEds =

Enter the tray numbers where feeds enter the column. Entries are in top-to-bottom order separated by commas.

Example: Total fractionator with 10 theoretical trays and three feeds:

There is a feed (stream 3) into the condenser, a feed (stream 2) to tray 6 and a feed (stream 1) to the bottom of the column. The location of the feeds would be entered as in the following command:

```
DIS10 = EXAM, 3, 2, 1, -4, -5, PAR, TRA = 10
LOCation of FEEds = 0, 6, 11
```

The condenser feed is considered to be to tray zero. If the feed to tray 6 is two-phase, the vapor portion will go to tray 5 and the liquid portion to tray 6. The vapor portion of the bottoms feed is to go to tray 10, therefore its location is entered as tray 11. The liquid portion of the bottom feed goes into the reboiler along with the liquid from the bottom tray. The liquid portion of this reboiler feed is not included in the column profile but is added to the bottom product.

Product Flowrates

PROduct rate (molar Q/t units or FRAction) =

Enter a molar guess for the top or bottom molar product rate and a specification for all side draw rates. The product rates must be in top-to-bottom order, separated by commas. Either the top or bottom product rate must be coded as zero, allowing an accurate overall material balance. To enter product rates as fractions of total feed to the column, specify FRA in the units option for this command.

NOTE: The nonzero top or bottom molar rate is used as a heat and material balance specification if the required number of specifications are not fulfilled (see *Distillation Heat And Material Balance Specifications*).

Molar flowrates must be entered for all side draws and are normally fixed. The addition of a RECover in SIDE draw n i command allows the program to vary the n th side draw rate until the specified amount of component i is recovered. A REFlux ratio (or REFlux FLOW) command is allowed in conjunction with the REC SID n i command. A nonmolar TOTAL PROduct SIDE n command also allows the program to vary the n th side draw rate until the specified amount of component i is recovered.

Example:

The PROduct command for the above column would be:

```
LOC SID = 0, -5, 10
PRO = 100, 1000, 50, 200, 0
```

where the 1000 LBMOL/HR side draw is from tray zero (the condenser), the 50 LBMOL/HR vapor side draw is from tray 5 and the 200 LBMOL/HR side draw is from tray 10. The top product rate is estimated as 100 LBMOL/HR and the bottom rate is calculated by subtracting all other product rates from the feed. Since this is a PARTial fractionator column type, two specifications are required (see *Distillation Heat And Material Balance Specifications*). If only one specification is entered, the top product rate of 100 LBMOL/HR will be used as the other specification.

Distillation: Convergence Algorithm

Four Convergence techniques are available: [Regular](#), [SUPER](#), [SUPER PLUs](#), and [SUM RATES](#).

Regular is always required if column type is either: ABS, ABS with PRESATurator, or ABS REB with PRESATurator. Regular is selected by default if TRAYS are 59 or fewer and all selected heat and material balance specifications are Regular (R) in table below. Also, the regular technique is the default for PROduct rate, REFlux ratio, TEMperature of CONDenser, or

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REBoiler duty specifications.

SUPer is selected by default if TRAYs are greater than 59 or at least ONE of the selected heat and material balance specifications is a SUPer (S) specification in the table below. SUPer and SUPer PLUs can be selected directly for use with any specifications by entering the SUPer or SUPer PLUs command.

SUM RATES is available to solve the Absorber and LLE columns using a three phase convergence technique.

Specification	Column Type					
	ABS REB	PRE SAT	STR	STR TOT	PAR	TOT
PRO	R	R	R	R	R	R
REF	-	-	R	R	R	R
REF FLO	-	-	S	S	S	S
TEM CON	-	-	R	-	R	-
DUT CON	-	-	R	R	S	S
TEM REB	R	R	-	-	S	S
REB	R	R	-	-	R	R
TOT PRO	S	-	S	S	S	S
PUR	S	-	S	S	S	S
REC	S	-	S	S	S	S
RAT	S	-	S	S	S	S
Inline FORTRAN	S	-	S	S	S	S

Regular (R) and SUPer/SUPer PLUs (S) specifications

Distillation: Heat and Material Balance Specifications

The performance of the DISTillation column is controlled by the heat and material balance specification. Values of the following variables can be specified:

- Reflux ratio or flowrate
- Condenser temperature or duty
- Reboiler temperature or duty
- Product composition - as a component purity, a component recovery, or a component ratio in the top, bottom, or side draw streams
- Product rates - top, bottom, or side draw.

Specifying columns with DESIGN II is easy. First determine the required number of specifications based on the column type from the table *Distillation Column Type Versus Number of Specifications Required*. Then simply enter the required number of specification commands from the choices detailed in *Distillation: Molar Product Rate Specifications*, *Distillation: Product Composition Specifications*, and *Distillation: Non-Molar Product Rate Specifications*. DESIGN II will automatically determine which column parameters to vary to meet your choice of specifications. For example, a PARTial condenser column type (column with partial condenser and a reboiler) requires two specifications. If the reflux ratio and bottom product molar flowrate are entered as specifications, then DESIGN II will vary the condenser and reboiler duties to meet the specifications.

Distillation: Column Type Versus Number Of Specifications Required

Choose the number of specifications required based on the column type.

Column Type	Number of Specifications Required
ABSORber	no specifications
ABSORber with REBoiler	1 specification
STRipper with partial condenser	1 specification
STRipper with TOTal condenser	1 specification
PARTial fractionator	2 specifications
TOTal fractionator	2 specifications

Distillation: Molar Product Rate Specification

The PROduct rate command must always be entered and the value of either the top or bottom product rate must be entered as zero. If the required number of specifications is fulfilled, the PROduct rate command is used as an initial guess.

The top or bottom product's molar flowrate entered as a guess on the required PROduct rate command will be used as a heat and material balance specification if the required number of specifications are not met with the specification commands below.

PROduct (molar Q/time into or FRA)=

Enter a molar flow rate for the top or bottom product and all side draw products. The product rates must be in top-to-bottom order, separated by commas. Either the top or bottom product rate must be coded as zero to allow an accurate overall material balance. For columns without side draws, the product rate can be entered as a fraction of the total feed to the column. Simply specify FRA in the units option for this command. E.G. PRO(FRA)= 0, .5.

This is particularly useful for recycle problems where the total feed rate to the column may be varying.

NOTE: Side draw product rates are normally treated as specifications and not as guesses. The two exceptions are for the RECOVERY SIDE and TOTAL PRODUCT SIDE draw commands.

For example, suppose the column type is an ABSorber with REBoiler, then 1 specification is required. If no specification command is entered, then the nonzero value for the top or the bottom flowrate entered on the PROduct rate command becomes the specification.

Distillation: Reflux Specifications

(only one of the following can be selected)

REFlux ratio =

Enter the reflux to total overhead product molar ratio. The total overhead product is vapor distillate plus liquid distillate. If the reflux ratio is not to be used as a specification, a guess can be entered with the optional REFLux GUEss command. (Column types: STR, STR TOT, PAR, TOT)

or

REFlux FLOWrate (Q units/t units) =

Enter the molar, mass, or volume rate of the liquid returning to tray one from the condenser. The SUPer or SUPer PLUs convergence option is required. (Column types: STR, STR TOT, PAR, TOT)

Distillation: Condenser and Reboiler Specifications

(only **ONE** can be selected)

TEMperature of CONDenser (T units) =

Enter the condenser temperature. (Column types: STR, PAR)

DUTy of condenser (H units/t units) =

Enter the condenser duty. The SUPer or SUPer PLUs convergence option is required. (Column types: STR, STR TOT, PAR, TOT)

TEMperature of REBoiler (T units) =

Enter the reboiler outlet temperature. The SUPer or SUPer PLUs convergence option is required except for ABS REB. (Column types: ABS REB, PAR, TOT)

REBoiler duty (H units/t units) =

Enter the reboiler duty. (Column types: ABS REB, PAR, TOT)

Distillation: Product Composition Specifications

Product specification may be made for a component purity, component recovery, or a component ratio in either the top, bottom, or side products. If these specifications are included in the input files, the SUPer convergence options is automatically used.

The product specification commands are listed below. Replace i and j with the desired component ID numbers *not* the order in the COMponent list. The error in meeting these specifications can be estimated on a RELative or ABSolute basis. RELative error is (calculated - specified)/specified. ABSolute error is (calculated-specified).

PURity in TOP (MOLar or MASSs, RELative or ABSolute) i =

Enter the fraction of component 'i' desired in the overhead product. MOLar fraction and RELative error options are defaults.

PURity in BOTtom (VOLume, RELative or ABSolute) i =

Enter the volume fraction of component 'i' desired in the bottom product. RELative error is the default option.

PURity in SIDE draw n (MOLar or MASSs, RELative or ABSolute) i =

Enter the fraction of component 'i' desired in the nth side draw product. MOLar fraction and RELative error options are defaults.

RECovery in TOP (MOLar or MASSs - Q/t units, RELative or ABSolute) i =

Enter the flowrate of component 'i' desired in the overhead product. LBMOL/HR and RELative error are the default options.

RECovery in BOTtom (units) i =

Enter the recovery in volume fraction of component 'i' desired in the bottom product. Use GAL/HR if STP units are needed.

RECovery in BOTtom (units) i =

Enter the recovery in volume fraction of component 'i' desired in the bottom product. Use M3/HR if NTP units are needed.

RECovery in SIDE draw n (MOLar or MASSs - Q/t units, RELative or ABSolute) i =

Enter the flowrate of component 'i' desired in the nth side draw product. LBMOL/HR and RELative error are the default options.

RATio in TOP (MOLar or MASSs, RELative or ABSolute) i,j =

Enter the fraction of component 'i' to second component j desired in the overhead product. MOLar ratio and RELative error are the default options.

RATio in BOTtom (VOLume, RELative or ABSolute) i, j =

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Enter the ratio of volume fraction of component 'i' to second component j desired in the bottom product. RELative error is the default option.

RATio in SIDE draw n (MOLar or MASS, RELative or ABSolute) i,j =

Enter the fraction of component 'i' to second component j desired in the nth side draw product. MOLar ratio and RELative error are the default options.

Example:

```
PURity TOP (MOL,REL) 23 = .996
```

This specification means that the purity of component number 23 (propylene) in the top product is 99.6 mole percent. If two product composition specification commands are entered, a weighting factor can be added to each (after the value) to indicated which specification is more important. For example,

```
PUR SID 1 (MOL,REL) 22 = .99987, 1.0  
PUR BOT (MOL,REL) 3 = .982, .5
```

The PURity SIDE n i and RATio SIDE n i, specifications are met without changing the total side draw flowrate. For these specifications the total side draw rates remain the same values as entered in the PROduct rate command. However, the RECOVERY SIDE n i specification is met by varying the total side draw rate from the value in the PROduct rate command if another specification such as REFLux ration has been entered.

Distillation: Non-Molar Product Rate Specifications

For non-molar (mass or volume) product rate specifications, use one or two of the following commands. The SUPer or SUPer PLUs convergence option is required. Do not specify both the top and bottom rates.

TOTAL PROduct TOP(Q units/t units) =

Enter the non-molar specification for the top product.

TOTAL PROduct SIDE n (Q units/t units) =

Enter the non-molar specification for the nth side draw product. Molar PROduct guess will be adjusted.

TOTAL PROduct BOTtom (Q units/t units) =

Enter the non-molar specification for the bottom product.

Distillation: Help on Specification Selection

Specification selection(s) depends on column type. The correct specification for your particular column depends on what you want and how difficult the column might be to solve. Some general guidelines for the selection of heat and material balance specifications are discussed on.

Run a shortcut: If either of the fractionator column types is selected (PAR or TOT), consider running a SHORtcut calculation on the column. See *Shortcut fractionator* Section. The SHORtcut output provides guesses for the top and bottom temperatures and the product rates. Also, the SHORtcut output can tell you when there may be a constraint that would prevent making the desired product. For example, you may be limited to a condenser temperature of 120 F, but the SHORtcut shows that a lower top product temperature is required to achieve the desired purity. Use of the SHORtcut allows adjustment of the column pressure before the rigorous (more expensive) calculation is performed. This calculation should not be used for non-ideal or azeotropic distillations.

Optimize only when necessary: When selecting heat and material balance specifications, remember that PURity, RECOVERY and RATio product specifications can be more difficult to converge than the other specifications. Use these specifications only when interested in optimizing your column to the desired product specification. The best approach is to converge the column first with easy specifications, then optimize it.

Easy specifications: For columns with two required specifications, convergence is normally faster for a reflux ratio and product rate specification. The TEMperature PROFILE, PROduct rates, or other useful information from the converged run might be used as input for subsequent runs to improve convergence.

Difficult specifications: Some specifications may cause difficulties in convergence, and selection of another specification may be necessary. The temperatures and vapor profiles from the run converged with the easier specification can be input as initial guesses for the run with the desired specification.

For columns requiring only one specification (ABS REB, STR, and STR TOT) care must be taken not to make an impossible specification. For example, if the REB duty for an ABSorber REBoiler is too large, all the liquid in the column would vaporize. For columns requiring two specifications, certain specification combinations can cause difficulties in convergence because one specification is related to the other. For example, if the heavy component PURity in the TOP product and the TEMperature of CONDenser are specified for a PARTial condenser, convergence will be almost impossible. The heavy component in the overhead product (PUR TOP) directly affects the dew point temperature (TEM CON). Care should be taken to select specification combinations that do not restrict each other. Another example is specifying the RECOVERY to the TOP product of the light key and then specifying the PURity in the BOTtoms of the same component. One specification may limit the other.

Distillation Optional Commands

Distillation: Side Draws

Up to seven of vapor or liquid side draw products can be specified with the LOCation of SIDE draws and PROduct rate commands (total of 9 products per column).

LOCation of SIDE draws =

Enter the tray number location(s) for the side draw(s) in top-to-bottom order, separated by commas. Positive tray numbers indicate a liquid draw. Negative tray numbers indicate a vapor draw. Liquid distillate draws for STR and PAR column types are indicated as side draws from tray zero.

Side draw flowrates must be specified on the PROduct rate command and are normally fixed. The side draw flowrate in the PRO command will be varied only to meet REcovery SIDE or TOTAl PROduct SIDE draw specifications. Outside the DISTillation module the side draw rate can be varied with a CONTroller equipment module or with Inline FORTRAN.

Example: LOC SID = 0, -5, 10

Distillation: Condenser Commands

PREssure out of CONDenser (P Units) =

Enter the pressure out of the condenser. Default is PREssure of TOP tray specified.

REFlux GUEss=

Enter an initial guess for the ratio of moles of liquid returned to the tray one to the total overhead product. Default guess is 3.

TEMperature out total CONDenser (T units) =

Enter the desired condenser temperature for TOTAl or STRipper TOTAl column types. If the specified temperature does not totally condense the overhead product, the bubble point temperature will be used for the condenser.

TEMperature CONDenser SUBcooling (T units) =

Enter the number of degrees of subcooling for TOTAl and STRipper TOTAl column types.

Distillation: Thermosiphon Reboiler Calculation

The command for specifying a thermosiphon reboiler is:

THERmosiphon vapor fraction =

Enter the mole fraction of the thermosiphon reboiler outlet stream that is vaporized.

Use this command to model a thermosiphon reboiler rather than the default kettle reboiler. Thermosiphon reboiler calculations are based on the following three assumptions.

- No mixing of return vapor and downcomer liquid.
- Pump work input is zero
- No heat losses in the reboiler system.

The bottom product will have the same composition as the circulating fluid. The product temperature will be between the bottom tray temperature and the returning vapor temperature. The circulation rate can be determined by the following equation:

$$F = V / \text{THE}$$

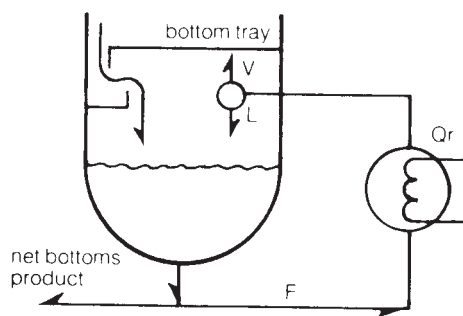
where

F = total flow to reboiler after bottom product is removed,

V = vapor returned to column in molar units,

THE = mole fraction vaporized.

The composition, but not the rate of the circulating fluid, is reported in the last stage of the tray-by-tray composition summary. PRInt SWItch = 2 is required to obtain this output.



Distillation: Decant Water and other Immiscible Components

A component (typically water) can be decanted from the condenser and/or any tray in the column. The decanted streams are **NOT** numbered on the flowsheet. The DEC COM command **without** the LOC DEC command will allow decanting from the condenser only. Use both the DEC COM **and** LOC DEC commands to decant from one or many locations including the condenser. All other commands are optional.

DECanting COMPONENT =

Enter the component ID number of component to be decanted. (For water, DEC COM = 62)

LOCation of DECants =

Enter the tray number(s), separated by commas, where the component is decanted. The condenser is tray zero.

Requires SUPER or SUPER PLUs convergence techniques, not for regular convergence techniques. For example: LOC

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DEC = 1,3 decants from trays 1 and 3; while LOC DEC = 0 decants only from the condenser.

DECant RATE guess (molar Q units/t units) =

Enter guess of the total decanted from the condenser (optional).

DECant in REFlux =

Enter mole fraction of decanted component dissolved in the reflux (optional). If this command is not entered when decanting water, the mole fraction of water will be calculated by the option selected in the **GENeral** section. The default solubility is based on the water-in-kerosene chart from the API Technical Data Book. See *Thermodynamics Section*.

This command can be used only with DEC COM option, not LOC DEC.

WATER FRAction =

Enter estimate for the amount of free water in the total liquid on the trays (fractional basis). Profile should begin at tray 0.

CALculate PHase =

Enter a 1 for every tray you want to have checked for free water, beginning with the condenser (tray 0).

IMMiscible =

Enter the component ID for water (IMM = 62) if the K-value option selected in the **GENeral** section does not automatically treat water as immiscible and immiscible treatment is desired. When decanting water, it is recommended that water be treated as immiscible. When using the DEC COM command **without** the LOC DEC command, the component can only be decanted from the condenser (for example: DEC COM = 62). In this case, the program will perform a rigorous calculation of the two liquid phases **only at the condenser**. In this case, a separate water phase will not be considered on the trays.

When using the DEC COM command **and** the LOC DEC command, the component can be decanted from the condenser and/or any tray (for example: DEC COM = 62, LOC DEC = 0,1,2, SUPER). If decanting water and using the LOC DEC command, the program will perform a rigorous calculation of the two liquid phases on all trays. The calculation assumes the water phase is pure water and that water is dissolved in the hydrocarbon phase to the extent predicted by the correlation selected by the user. The default solubility is based on the water-in-kerosene chart from the API Technical Data Book. See *Thermodynamics Section*.

The amount of component decanted from the condenser should not be included in your specification or estimate of overhead product rate which is entered on the **PROduct** rate command. For decant from the condenser of a second liquid phase which contains more than one component, do not use the decant commands. Consider using separate **HEAt EXChanger** and **MULTIPHase** flash (rigorous 3-phase flash) modules to model the condenser. Appropriate *K-Value Options* with *ChemTran* regressed VLE, VLLE or LLE data, such as **RENon** or **UNIQUEACK**, should be used.

Distillation: Extractive (Entrainer) Column Calculations

EXTractive COMponent =

Enter the component ID number of the extractive component in gasohol or extractive columns. Only one extractive component is allowed per column. Requires **SUPer** convergence technique. Benzene, diethyl ether, and pentane are typical entrainers for the ethanol-water system.

Distillation: Tray Heaters and Coolers

Heaters

Besides the condenser and reboiler, an essentially unlimited number of heaters and coolers can be added on any tray in the column. Enter both commands to locate heaters/coolers and specify their duties.

LOCation of HEAters or coolers =

Enter the tray number(s) where the heater(s) and cooler(s) are located. The tray number(s) are entered from top to bottom and separated by commas.

and

HEAt (H units/t units) =

Enter the duties for heaters and coolers in the same order as in the LOC HEA command. Use positive values for heating and negative values for cooling. The specified duty is applied directly to the designated tray. The liquid and vapor to the designated tray are mixed and the specified enthalpy added or subtracted. The **DIStillation** module then calculates the resulting temperature and vapor-liquid equilibrium split.

Example:

```
LOC HEA = 56
HEA (BTU/HR) = 2.3 E6
```

A heater is located on tray 56 and adds 2.3 million BTU/HR heat to that tray.

Example:

```
LOC HEA = 3, 6, 18
HEA (BTU/HR) = -15 E6, -22.5 E6, 7.1 E6
```

These commands show 15 E6 BTU/HR cooling on tray 3, 22.5 E6 BTU/HR cooling on tray 6, and 7.1 E6 heating on tray 18.

Intercoolers

Use intercoolers to selectively cool or heat either the liquid or the vapor leaving a tray to a specified temperature and return it to the column.

Enter only two commands to define all intercoolers. Always enter the LOCATION of INTERcoolers command and enter one of the cooling specifications: TEM INT, DUT INT, or DEL TEM INT.

LOCATION of INTERcoolers =

Enter the tray number(s) to specify that either the liquid (positive tray number) or the vapor (negative tray number) from that tray is to be cooled or heated. Liquids are returned to the tray below. Vapors are returned to the same tray. The tray number(s) are entered from top to bottom and separated by commas. Vapor draws require SUPER convergence option.

TEMPerature out of INTERcoolers (T units) =

Enter the temperature(s) out of intercooler(s). Enter one value for each intercooler location, separated by commas, in top-to-bottom order.

DUTy of INTERcoolers (H units/t units) =

Enter the duty(s) of intercooler(s). Enter one value for each intercooler location, separated by commas, in top-to-bottom order. Duty is positive for heating and negative for cooling. Requires SUPER convergence option.

DELta TEMperature of INTERcoolers (T units) =

Enter the temperature changes for intercooler(s). Enter one value for each intercooler location, separated by commas, in top-to-bottom order. Requires SUPER convergence option. Intercoolers and heaters can significantly affect tray temperature and vapor traffic. Entering temperature and/or vapor profiles may help convergence. See *Rigorous Distillation Column Profiles* for details.

DUTy of INTERcooler GUEss (H units/t units) =

Enter a guess for the heat added to or removed from each intercooler in top to bottom order.

TEMPerature of INTERcooler GUESS (T units) = Enter an estimate for the intercooler return temperatures.

Example:

```
LOC INT = 5, -10
DUT INT = -5E6, -0.4E6
```

The liquid from tray 5 is cooled by 5E6 BTU/HR and returned to tray 6. The vapor from tray 10 is cooled by 0.4E6 BTU/HR and returned to tray 10.

Distillation: Column Efficiency

In order to approach more closely the actual operating conditions within a column, efficiencies for mass and heat transfer are needed for conventional column simulations. DESIGN II can perform a "modified vaporization efficiency" on the entire column. This is a simplified approach based on Holland & Welch's version ("Steam Batch Distillation Calculation," Petroleum Refiner, 36, No.5, 251 (1957)). They modified the original definition of "vaporization efficiency" by McAdams (Chemical Engineers Handbook, 3 ed., J. H. Perry).

All commands are required and optional. If you do not want to use the efficiency commands, results will be based on the specified theoretical trays of the column.

EFFiciency of COLumn =

Enter the desired column efficiency applied for all trays (except condenser & reboiler). Default is 1.0.

EFFiciency of BASE component i =

Enter the efficiency of the base (heavy key) component in the mixture. "i" is the DESIGN II component ID number. Default is 1.0.

Calculation Method:

Modified Vaporization Efficiency (i) = Efficiency of Base component * {Relative Volatility (i) ** (Efficiency of Column - 1.0)}

Modified K-value (i) = Modified Vaporization Efficiency (i) * K-value (i) where, Relative Volatility (i) = K-value (i) / K-value (base component) and "i" – any component

Notes:

1. The commands can be used only for DISTillation columns and not for REFine columns.
2. Both commands have to be used together (via Column Efficiency dialog or Keyword Input)
3. Only one "EFF BAS i" command and component can be used. Care should be exercised on the choice of heavy key component.
4. If you specify a column efficiency of less than 100 percent then it should be noted that this will affect the internal flow rates of the trays, the temperature of each stage, and the value of the condenser and reboiler duties. Thus these values may not agree with equivalent values that have been calculated with an external set of unit modules even though these unit modules use Internal Reboiler/Condenser streams as feed streams.

Distillation: Tray Sizing

There are two different shortcut sizing techniques in the DISTillation column calculations. Both calculations are performed

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automatically using default values unless you enter one or more of the commands listed below.

Smith-Dresser-Ohlswager Technique

The first is the Smith-Dresser-Ohlswager technique (Smith, R.B., Dresser, T. and Ohlswager, T., *Hydrocarbon Processing*, Vol. 40, No. 5., pp. 183- 184 (1963)). This correlation calculates the column diameter at 100 percent of flood.

The method is general for bubble cap, sieve and valve trays and is therefore subject to considerable error and should not be used for final column design. The correlation has limits for the liquid to vapor ratio and warning messages indicate when the limits are exceeded.

All commands are optional. If you do not want to use the default 18 inches settling height, you must enter all of the following commands:

SPACING of TRAYS (L units)=

Enter the tray spacing to be used along with WEIR HEIGHT and WEIR LENGTH in calculating the settling height. Default is 18 inches settling height.

WEIR HEIGHT (L units)=

Enter the WEIR HEIGHT to be used along with SPACING of TRAYS and WEIR LENGTH in calculating the settling height.

WEIR LENGTH (L units)=

Enter the WEIR LENGTH to be used along with SPACING of TRAYS and WEIR HEIGHT in calculating the settling height.

DOWNCOMER AREA (L2 units) =

Enter the downcomer area in square feet. Default is 12 percent of the empty column area.

Values entered with the SPACING of TRAY, WEIR HEIGHT, and WEIR LENGTH commands are used in calculating the settling height (tray spacing minus clear liquid depth). If any one of these three commands is not entered, the settling height is assumed to be 18 inches. Minimum settling height is 2 inches and maximum is 30 inches for the correlation. DOWNCOMER AREA is used in calculating the vapor velocity on each stage. If not entered, the DOWNCOMER AREA is set to 12 percent of the empty column area.

Glitsch Technique

The second sizing technique is provided in cooperation with Glitsch Incorporated (Glitsch Bulletin 4900, Design Procedure for Ballast Trays). This shortcut method was developed for ballast trays but is also applicable for sieve trays with 14% hole area. This technique is applicable for tray spacings of 12-48 inches and percent of flood values from 20-100%.

By default the Glitsch, Inc. correlation calculates column tray diameters at 70% - 80% of flood based on tray loadings, system factor and tray spacing. The number of passes will be calculated if you do not specify a value. You can specify a different percent of flood with the GLITSCH PERCENT FLOOD command.

Optionally, specify the GLITSCH DIAMETER and the percent of flood will be calculated. Do not specify both GLITSCH DIAMETER and GLITSCH PERCENT OF FLOOD.

GLITSCH SYSTEM factor =

Enter the system factor for foaming on the trays. Default is 1.0 which is appropriate for non-foaming, regular systems. One input value allowed.

GLITSCH PERCENT FLOOD=

Enter the percent of flood for the column. If not specified, the program will calculate. One input value allowed.

GLITSCH PASSES per tray per section=

Enter the number of tray passes. If not specified, the program will calculate. One input value allowed: 1, 2, or 4 passes. In REFINED columns only, GLITSCH PASSES can be different and should correspond to the number of GLITSCH SWAGE TRAYS plus one.

GLITSCH SPACING per tray per section (L units) =

Enter the spacing(s) of trays. Default is 2 feet. The technique is valid for tray spacings from 1 to 4 feet. See GLITSCH SWAGE command for additional capability.

GLITSCH DIAMETER per tray per section (L units) =

Enter the column diameter(s). If not specified, the program will calculate. You cannot specify both GLI DIA and GLI PER. See GLITSCH SWAGE command for additional capabilities.

GLITSCH SWAGE TRAYS =

Enter the tray numbers immediately below the swage in the column. The GLITSCH SWAGE command can be used in conjunction with either GLITSCH DIAMETER or GLITSCH SPACING of trays or both for columns with more than one diameter or tray spacing. The GLITSCH SWAGE command will have one less value than the GLI DIA or GLI SPA commands.

GLITSCH DOWNCOMER AREA per tray per section (L2 units) =

Enter the downcomer area per tray. Will be calculated, when not provided.

GLITSCH WEIR HEIGHT per tray per section (L units)=

Enter the WEIR HEIGHT to be used along with GLITSCH SPACING in calculating the settling height. Default is 3 inch.

GLITSCH VALVE TYPE = 1 or 4

Enter the valve type. Either 1 or 4 is available (per Glitsch Bulletin 4900). Default is 1.

V-1 A general purpose standard size unit, used in all services. The legs are formed integrally with the valve for deck

thicknesses up to 3/8"

V-4 This signifies a venturi-shaped orifice opening in the tray floor which is designed to reduce substantially parasitic pressure drop at the entry and reversal areas. A standard ballast unit is used in this opening, normally, although a V-2 or V-3 unit can be used for special services. The maximum deck thickness permissible with this opening is 10 gage.thickness permissible with this opening is 10 gage.

GLItsch VALve MATerial =

Enter the valve material. Default is carbon steel.

Material

Keyword in bold

ALUMinum

CARBon steel (default)

COPPer

MONEl

NICKel 200

HASTalloy

STAINless steel 304

LEAD

TITANium

GLItsch VALve THickness (L units) =

Enter the valve thickness. Default is 0.06 inch.

GLItsch VALve NUMber (1/L2 units) =

Enter the number of valves per square foot of active area. Default is 13.

GLItsch DECK thickness (L units) =

Enter the deck thickness. Default is 0.104 inch.

It is important to use the correct system factor (GLI SYS =) for foaming on the trays. The default value used by the program is 1.00, which is appropriate for non-foaming, regular systems. Other recommended values for GLItsch SYStem factor are as follows:

System	Value
Lean oil absorbers, amine & glycol regenerators (moderate foaming)	0.85
Amine & glycol contactors (heavy foaming)	0.73
MEK units (severe foaming)	0.60
Caustic regenerators (foam-stable)	0.30

The GLI SYS, GLI PER and GLI PASses commands are limited to one value per distillation column. The GLItsch SPAcing and GLI DIAMeter commands are allowed multiple values. Use the GLItsch SWAge command to tell the program where the different diameter/spacing sections begin. Values are entered in top-to-bottom order.

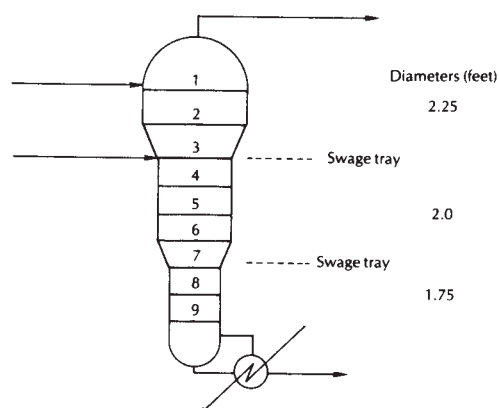
Example: Multiple diameters

This demethanizer has two swages resulting in three different column diameters. The commands:

GLItsch SWAge trays = 3, 7

GLItsch DIAmeters = 2.25, 2, 1.75

define the theoretical tray below each swage and the three column diameters.



Distillation: Calculation Options

CO2 FREeze

Enter this command to check whether solid CO2 will form at any of the tray conditions in the column (typically for cryogenic natural gas mixtures).

Condenser and Reboiler Curves

CONDensing **CUR**ve

Enter this command to get a cooling curve for the vapor leaving the top tray for any column type containing a condenser. The temperature range of the cooling curve is from the top tray temperature to the condenser outlet temperature. If a PREssure of CONDenser command has been entered, equal delta pressure increments will be used.

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REBoiler CURve

Enter this command to get a heating curve for the liquid leaving the bottom tray for any column type containing a reboiler. The temperature range of the heating curve is from the bottom tray temperature to the reboiler outlet temperature.

Distillation: Internal Stream Commands

Internal streams are very useful when it is required to view the results of a stream that are internal to the DISTillation Column after a column has been converged. The details of streams going in and out of column components such as condenser, reboiler, side heater or cooler is easily obtained by using these commands. Information on temperature, pressure, and flow of each component is accessed and is displayed in the stream summary and detailed stream summary sections. Note that the numbers used for these streams should not be on the flowsheet except for those specified as products or sidedraws. Specific internal stream commands are listed below.

Condenser Internal Streams

CON STR = x, -y

Enter this command for columns with condensers (PAR, STR, TOT, STRTOT, PRESAT) where x is a stream number assigned to the tray 1 vapor and y is a stream number assigned to the product to the reflux accumulator.

CON SEP STR = x, -y

Enter this command for columns with condensers (PAR, STR, TOT, STR TOT) where x is a stream number assigned for the vapor leaving tray 1 at the condenser outlet conditions and stream number 'y' is assigned to the stream refluxed back to the main column excluding any liquid distillate and decanted water.

Reboiler Internal Streams

REB STR = x, -y, -z

Enter this command for columns with kettle reboilers (PAR, TOT, and ABS REB) where x is a stream number assigned to the bottom tray liquid, y is a stream number assigned to the vapor return, and z is the stream number assigned to the bottoms product.

REB STR = x, -y

Enter this command for columns with thermosiphon reboilers (THE command is present) where x is a stream number assigned to the reboiler feed and y is a stream number assigned to the reboiler return.

Side heater internal streams

HEA STR i = x, -y

Enter this command for columns with side heaters. 'i' represents the tray location above the tray where the heat is added to/removed from the column; 'x' represents the composition of the liquid stream leaving the tray above the tray specified in the LOC HEA command; 'y' represents the stream entering the tray where the heating/cooling is applied. For example LOC HEA=3, HEA=10E6, HEA STR 2=5,-6.

Intercooler internal streams

INT STR i = x, -y

Enter this command for any with intercoolers where i is the tray number, x is a stream number assigned to the intercooler feed, and y is a stream number assigned to the intercooler return.

NOTE: The stream numbers used for internal streams should not be connected to other external process equipment modules. You can use the Inline FORTRAN COPSTR (i, j) function to copy the stream composition to another stream for additional calculations. See Inline Fortran: Table 5. Utilities Subroutines (use with CALL) for more details

You may use CON SEP STR command with CON CUR and with CON STR commands. CON SEP STR command does not work with PRE SAT columns (use PAR or STR instead).

Distillation: Feed Phase Commands

Enter the BUBble point or DEW point commands to force the program to calculate the correct feed temperature at the feed tray pressure for any feed stream. Enter the LIQuid or VAPor commands to force the calculation of the feed enthalpy to be for a single phase, regardless of the feed flash results. For any of the commands, use the stream number from the flowsheet to identify for which streams this is to occur.

BUBble point =

Enter the stream number(s) for the streams which are to enter the column at the bubble point temperature and feed tray pressure.

DEW point =

Enter the stream number(s) for the streams which are to enter the column at the dew point temperature and feed tray pressure.

LIQUid =

Enter the stream number(s) for the streams whose enthalpy will be calculated as liquid for the stream temperature(s) at the tray pressure(s).

VAPor =

Enter the stream number(s) for the streams whose enthalpy will be calculated as vapor for the stream temperature(s) at the tray pressure(s).

Distillation: General Lost Work Calculations

If a LOST work command is entered in the GENeral section of the input, you may enter the following commands to change defaults for the exchange temperatures for the condenser, reboiler, heaters/coolers, and intercoolers.

TEMPerature of HEAting fluid (T units) =

Enter the value for the utility side fluid temperature of the reboiler or side heaters to be used in the LOST WORK analysis. Default is 250 F.

TEMPerature of COOLing fluid (T units) =

Enter the value for the utility side fluid temperature of the condenser or intercoolers to be used in the LOST WORK analysis. Default is 70.3 F.

The results for the LOST WORK analysis are not reported in the distillation column output. They appear in a separate report which is printed immediately before the detailed stream summaries.

Distillation: Thermodynamics Commands

IMMiscible =

Enter the component ID number of the immiscible component. If the K-value does not automatically treat water as immiscible and immiscible treatment is desired, enter IMM = 62. When decanting water, it is recommended to treat water as immiscible. See *Thermodynamics: Water K-Values in Hydrocarbon Systems*, for immiscible component guidelines.

NO IMMiscible

Enter this command to have water treated miscibly for K-value options which normally treat water immiscibly. Not allowed when decanting water. See *Thermodynamics: Water K-Values in Hydrocarbon Systems*

Distillation: Print Options

Tray Sizing Print Options Choose *one* of the following commands to select which sizing correlation output you wish, if any:

SMIth SIZing OFF

Enter this command to delete the Smith-Dresser-Ohlswager calculation and output.

GLItsch SIZing OFF

Enter this command to delete the Glitsch sizing calculation and output.

COLumn SIZing OFF

Enter this command if no column sizing output is desired in the program output.

NOTE: The default PRInt SWItch command automatically produces both sets of tray sizing output. PRI SWI = 0 also suppresses the tray sizing calculations.

Plotted Output

PLOt OFF

Enter this command to eliminate the following DISTillation column plots: enthalpy versus temperature for reboiler and condenser curves, separation parameter profile, vapor-liquid traffic profile and vapor-liquid mole fraction profile for light and heavy key components.

Control Column Output

The PRInt SWItch command controls the amount of distillation column output. Selecting the appropriate switch option allows as much or as little of the column calculations to appear in the output. To minimize column output, use PRI SWI = -2. To get full details, use PRI SWI = 2 or 3.

A value of -1 for PRI SWI minimizes column output during recycle calculations. When the recycle loop is converged (or the iteration number equals the value you have entered on a GENeral section PRI FRE command) full column results will be printed. The function of each PRInt SWItch option is listed below.

PRInt SWItch =

- | |
|--|
| Enter desired PRInt SWItch option number from the following table. Default is 2. |
| -2 Enter this PRI SWI for minimum output. |
| -1 Enter this PRI SWI when the DISTillation column is in a recycle loop and you want the detailed tray-by-tray printout and column sizing for the last (or converged recycle) recycle loop iteration only. |
| 0 Product component flowrates and properties are printed along with the column heat and material balance errors for each iteration during column convergence. Temperature profiles are printed along with the following properties for both the liquid and vapor on each stage: |
| - molar flowrate |
| - mass flowrate |
| - molecular weights |
| - viscosities |

- densities
 - specific gravities
 - enthalpies
 - surface tension
- 1 In addition to PRI SWI = 0 information, two shortcut column sizing calculations are printed: Smith-Dresser-Ohlswager and Glitsch. Actual gallon-per minute and feet-per-second vapor velocities are printed for each stage. Tray-by-tray temperatures, K-values and mole fraction compositions are also printed. This option will also give detailed column output when the number of the recycle loop iteration matches the value specified in the PRI nT FREquency command in the GENeral section.
 - 2 In addition to PRI SWI = 1 information, plots of the tray temperature profile, separation parameter, and liquid and vapor profiles are printed.
 - 3 The same information as PRI SWI = 2 is printed, except that the vapor and liquid tray-by-tray compositions are given as molar flowrates instead of mole fractions.

Identify Light And Heavy Keys

LIGHT KEY = and

HEAVY KEY=

Enter the component ID numbers of the light key and heavy key components to get a plot of light and heavy key component mole fractions in the vapor and liquid for each stage of the column.

The light and heavy key components specified will also be used in the separation parameter plot if PRI SWI = 2 or 3.

Separation Parameter Plot

The plot of separation parameter is presented at the end of the column output for PRI nT SWItch = 2 or greater. The plot is used to optimize feed tray location and theoretical trays for a desired light and heavy key-component separation. The plot is used mainly for TOTal and PARTial fractionator column types with a single feed. The separation parameter plot for multi-feed fractionators and other column types may be of some use but the results must be analyzed carefully to take into account the column configurations and feed information.

The separation parameter variable, which is printed at the extreme left of the separation parameter plot, is defined as $\ln X_{lk} / X_{hk}$ for each tray. X_{lk} is the liquid mole fraction of the light key component and X_{hk} is the liquid mole fraction of the heavy key component. The separation parameter variable is a measure of separation on any tray. The following column types with an additional feed to the middle of the column also can have a useful separation parameter plot: ABSorber, ABSorber REBoiler, STRipper, and STRipper TOTal. These configurations, although not true fractionators, can perform the same function. For example, the ABSorber, with a top liquid feed (like a reflux) and a bottom vapor feed (like the reboiler vapor) and a middle feed, could be similar to a fractionator. The same may be true for the ABSorber with REBoiler, STRipper and STRipper TOTal options. For the TOTal and PARTial fractionator type columns with single feeds, the separation parameter plot might look like one of the following three figures:

Figure 1 is typical of a column where the feed tray is located too low, while Figure 2 is typical of a feed tray located too high. These conditions are indicated by the relatively sharp breaks at the feed tray locations on the separation parameter plot. In order to relocate the tray at a more nearly optimum position, it is necessary to extrapolate one portion of the curve. If the tray is too low, you should extrapolate the curve below the feed as shown in Figure 1. If the tray is too high, you should extrapolate the portion of the curve above the feed as shown in Figure 2. The slope of the extrapolated curve will be equal to the slope of the other curve at some new tray location. This new location will be closer to optimum for the feed to this column.

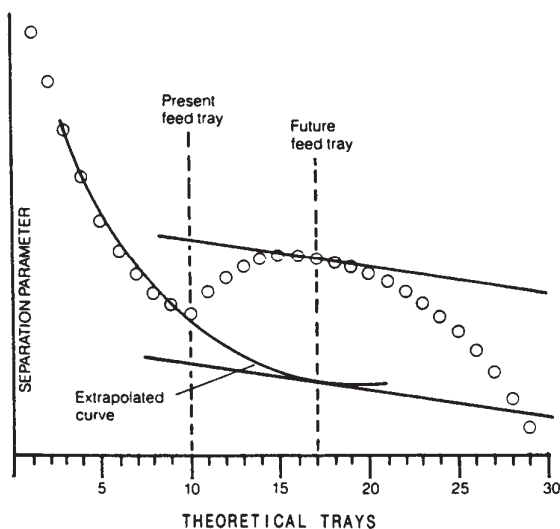


Figure 1 - Feed tray located too low

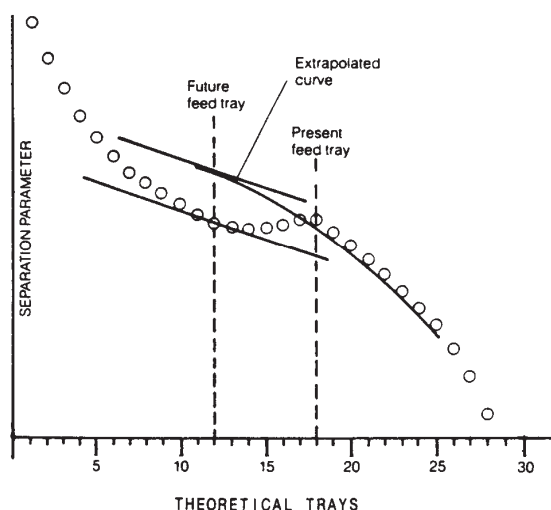
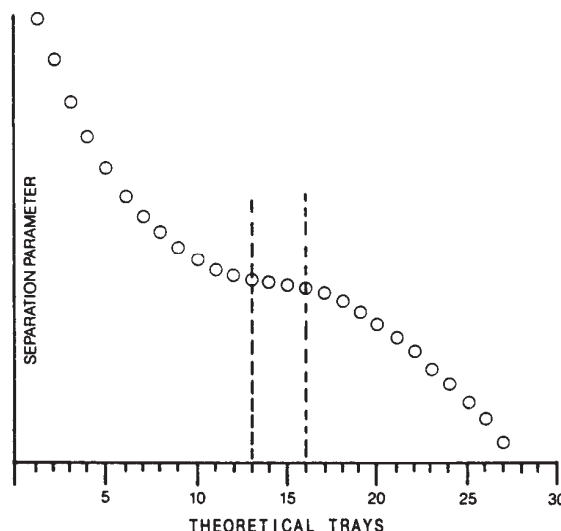


Figure 2 - Feed tray located too high

A nearly ideal separation parameter plot looks similar to Figure 3:

If the flat portion of the curve (between the dotted lines) contains several trays, the feed tray could be located at any one of them with little change in separation. Ideally, the flat portion of the curve would contain only one tray which would be the optimum feed location.



Distillation: Column Profiles

All profile commands are optional. The DISTillation module automatically sets up temperature and vapor profiles from your guesses of top and bottom product temperatures and flowrates. In some cases though it may be beneficial to enter your own estimates. Therefore, entry of tray-by-tray profiles for temperature, vapor traffic, liquid composition, and pressure are allowed. The first three types of profiles provide initial estimates for column calculations. Only the values entered for the PRESSure PROFILE remain fixed throughout calculations. Poor estimates for vapor or temperature profiles can cause nonconvergence.

TEMPerature PROFILE guess (T units) =

Enter a temperature guess for each tray in the column in top-to-bottom order separated by commas. Zeroes between temperatures are to indicate straight line interpolation for the tray temperature listed as zeroes. See *Distillation: Temperature Profile* Details for examples.

VAPor PROFILES (molar Q units/t units) =

Enter a vapor rate guess for each tray in the column in top-to-bottom order separated by commas. Zeroes between vapor rates are to indicate straight line interpolation for the tray vapor rates listed as zeroes. VAPor PROFILES usually are not needed with SUPER since they will be calculated by the program. See *Distillation: Vapor Profile* Details for examples.

REBoiler VAPor GUEss (molar Q/t units) =

Enter a guess for the vapor rate leaving the reboiler. This command is used in conjunction with the VAPor PROFILE command.

LIQuid COMposition profile i =

Enter the liquid mole fraction for component i for each tray in the column in top-to-bottom order separated by commas. Zeroes between values indicate straight line interpolation. This command should be used only with the regular distillation technique (not SUPER or SUPER PLUs) for unusual situations, such as highly nonideal systems with nonlinear composition profiles. Do not use with the COM CON convergence control command. See *Distillation: Liquid Composition Profile* Details for examples.

PRESSure PROFILES (P Units) =

Enter the desired pressure for each tray in the column in top-to-bottom order separated by commas. Zeroes between pressures are to indicate straight line interpolation for the tray pressures listed as zeroes. See *Distillation: Pressure Profile* Details for examples.

PRESSure of BOTtom (P units) =

Enter the pressure of the bottom product. Use command only if the PRESSure PROFILE command is also used.

NOTE: All of the above profiles can be retained and saved between every recycle loop and iterations. Please see *Distillation: Save Profile* details for specific commands.

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Distillation: Temperature Profile

DESIGN II initially estimates a linear temperature profile for all columns except reboiled absorbers using the regular convergence technique which sets up a quadratic profile. However, in some instances, the column temperatures may not follow a smooth profile. Typical examples of nonlinear temperature profiles are when feed temperatures are significantly higher (or lower) than the corresponding tray temperatures and when side heater/coolers or tray intercoolers are used.

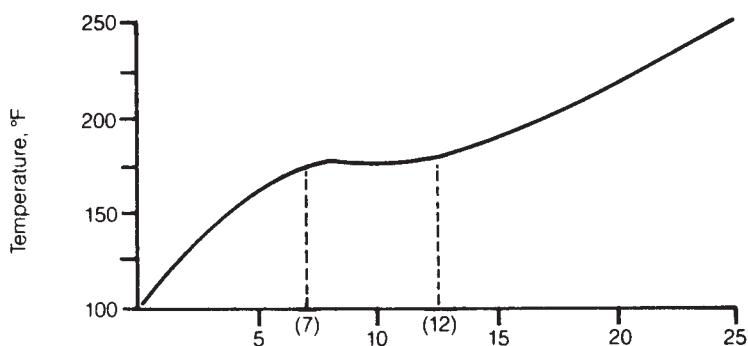
Example:

Enter the temperature profile shown in this figure. Use straight line interpolation between trays 1 and 7 and between trays 12 and 25. Repeat the temperature of 175 F for trays 7 through 12.

A guess for the above profile can be entered as:

```
TEM PRO = 100, 5*0, 6*175, 12*0, 250
```

If the temperature profile is not linear, there are two approaches for entering appropriate profile information in your input file. First, you can enter values for the top and/or bottom temperatures which are different from the actual product temperatures. For example, the temperature profile for a typical amine regenerator is reasonably linear from tray one through the reboiler. From tray one to the condenser, there is typically a temperature drop of 60 to 120 F. Entering TEM TOP = 200 rather than TEM TOP = 120 (the expected condenser temperature) will typically result in a converged solution. This procedure is also useful for sour water strippers and TOTal fractionators. Second, you can enter the profile for the entire column. ABSorber calculations rarely require temperature profiles. If heaters or intercoolers are added to the column configuration, a TEM PRO command can help convergence.



For most ABSorber with REBoiler column types without side heaters, the temperature profile is linear from tray one to the bottom tray. The major change in column temperatures occurs between the bottom tray and the reboiler. The addition of side heaters tends to make the temperature profile more linear. If you have one or more side heaters for an ABS REB column type, you can enter an abbreviated TEMperature PROfile which will cause the program to start calculations with a linear rather than quadratic temperature profile.

Example: If you have an ABSorber with REBoiler column type with a side heater, seven trays, an estimated top tray temperature of -140 F, and bottom tray temperature of 60 F, you would enter the following command to get a linear temperature profile rather than the default quadratic profile:

```
TEM PRO = -140, 5*0, 60
```

Distillation: Vapor Profile

The vapor profile estimated by the program takes into account vapor introduced by feeds. The initial vapor rate from the reboiler is generated from the values you enter for PRO and REFlux (if any). When you enter a VAPor PROfile for a column which has a reboiler, you should also enter a REBoiler VAPor GUEss command. If you do not enter a REB VAP GUE command with the VAPor PROfile command, DESIGN II will use the last value from the vapor profile as an estimate of the vapor flow from both the bottom tray and the reboiler.

Side heaters, intercoolers, and large composition differences between feeds and the trays they enter can significantly affect the vapor traffic in a column. You may wish to enter a VAPor PROfile if your column configuration contains any of these.

When using the SUPer or SUPer PLUs convergence techniques, a VAPor PROfile is not normally needed.

NOTE: Temperature profiles primarily affect material balance while vapor profiles control enthalpy balance.

Example: Enter a vapor profile for an 8 tray STRipper column type (column with partial condenser and no reboiler). Cold feed enters on tray 1 dropping the vapor rate from tray 1 and causing a significant change in the vapor profile. In this case a vapor profile may help convergence but it is not always necessary for convergence.

```
VAP PRO = 411, 695, 5*0, 725  
LOC FEE = 1,9  
TRAY = 8, STRIPPER
```

Distillation: Liquid Composition Profile

Liquid composition profiles are primarily used for highly nonideal, composition dependent systems such as amine contactors, sour water strippers, and some chemical systems. Liquid composition profiles can be entered for one or more components in a DISTillation column. The liquid composition profile for each component is entered on a separate LIQ COM i command, where i is the component ID number.

If you do not enter a COM CON command in the input file for an amine contactor and you enter a flow for the acid gas in the lean amine feed, DESIGN II will automatically estimate liquid composition profiles for the acid gas.

The LIQ COM command should not be used with SUPer or SUPer PLUs and should not be used with the COM CON convergence control command.

Example: Enter liquid composition profiles for CO₂ and H₂S for an MEA contactor.

```
LIQ COM 49 = 5*.0062, .0064, .018, LIQ COM 50 = 5*.12E-03, .3E-3, .32E-3, TRAY = 7
```

Distillation: Pressure Profile

DESIGN II normally uses values entered for PREssure of TOP tray, PREssure of CONDenser and DELta pressure to calculate a pressure profile for your column which will be linear from tray one through the reboiler (if any). Use a PREssure PROfile command to enter a pressure value for every tray in the column in top-to-bottom order, separated by commas. Values for the condenser and reboiler (if present) should be entered with the PREssure of CONDenser and PREssure of BOTtom product commands respectively. If you do not enter values for PRE CON and PRE BOT, DESIGN II will use the first and last values entered on your PREssure PROfile for the condenser and reboiler pressures.

Example: Enter a pressure profile for all trays and for the condenser and reboiler.

```
PRE PRO (MMHG) = 25,30,50,75,90
PRE CON (MMHG) = 10, PRE BOT (MMHG) = 100
TRAY = 5, PARTIAL
```

Distillation: Save Profile

Save Profiles Between Recycle Iterations

The SAVE PROfile, SAVE TEMperature, SAVE VAPor, and SAVE LIQuid profile commands are useful when the column is inside a recycle or controller loop. Profiles from converged columns are saved each iteration of the loop and are used as initial starting profiles for the column on subsequent iterations of the loop. It is a good idea to make sure columns within loops will converge before allowing the iterative calculation to proceed. This is best accomplished by running only one recycle loop iteration (MAX = 1, entered in the GENeral section).

SAVE PROfiles

Entered to have pressure, temperature, vapor, and liquid profiles saved between recycle and controller loop iterations.

SAVE TEMperature profiles

Entered to have temperature profiles saved between recycle and controller loop iterations.

SAVE VAPor profiles

Entered to have vapor profiles saved between recycle and controller loop iterations.

SAVE LIQuid profile

Entered to have liquid profiles saved between recycle and controller loop iterations.

SAVE MATrix

Entered to have the column matrix saved between recycle and controller loop iterations. This can significantly reduce computation time in flowsheet recycle cases. Do not use this command with the SUPer or SUPer PLUs convergence options.

Distillation: Run Shortcut Automatically

The DISTillation module automatically runs the shortcut distillation first if the column has a partial or total condenser. The light and heavy key components should be identified and fractions specified.

Identify Light And Heavy Keys

LIGHT KEY =

and

HEAVY KEY=

Enter the component ID numbers of the light key and heavy key components to get a plot of light and heavy key component mole fractions in the vapor and liquid for each stage of the column.

The light and heavy key components specified will also be used in the separation parameter plot if PRI SWI = 2 or 3.

FRAction LIGHT Key =

Enter the fraction (mass or molar) of the light key for the Distillation column to perform shortcut distillation calculations to provide top and bottom estimates of temperature and pressures.

FRAction HEAVY Key =

Enter the fraction (mass or molar) of the heavy key for the Distillation column to perform shortcut distillation calculations to provide top and bottom estimates of temperature and pressures.

NOTE: Both the light and heavy key commands are required

Distillation: Regular Convergence Technique

Enter any of the following commands to adjust the regular convergence control parameters. The default values are satisfactory for most runs and have been set to converge normal columns in the least amount of time. For nonideal columns consider adjusting the COM CON parameters first, then the DVS and DTS parameters, and finally the T STep parameter. The SAVE MATrix command is also useful for columns inside recycle or controller loops. It can save significant computational time for DIS after the first iteration of the recycle loop. Do not use this command with SUPer or SUPer PLUs convergence options.

TOLerance =

Enter the maximum acceptable NORM for the column. The NORM is the error in the tray heat and material balance on a fractional basis squared. The default is TOL = 0.1 E-4 or about 0.3% average error.

The square root of the NORM gives an approximation of the fractional error in heat and material balance, about 0.003 for the default. To have the balance within about 0.001(.1%) a TOL = 0.1E-5 is entered. For recycle loop calculations involving distillation columns where PROduct rate is not a specification, recycle loop convergence usually can be speeded up by changing the TOLerance to 0.1E-5.

MAXimum MATrices =

Enter the maximum number of matrix inversions for column solution. Default is 6.

Most columns, unless the specifications are difficult to meet, require no more than two matrix inversions. For larger columns (greater than 15 trays) you may wish to set the maximum number of matrices to two on the initial run to ensure a reasonable run time if the column has difficulty converging. The default value is MAX MAT=6, which means a nonconverged column could use up to 3 times more computer time than if you ran with a MAX MAT=2. If the column does not converge, but seems to be going in the right direction as measured by the NORM, the temperature and vapor profiles from the first run can be entered as starting guesses for the second run (TEM PRO= and VAP PRO=).

COMpositional CONvergence =

To stabilize compositional dependent K-values enter two number separated by commas. The first is the number of K-value iterations during each internal iteration. The second determines where in the column calculation scheme these internal K-value iterations occur: = 1 during Updates only; = 2 during Updates and Matrix recalculations; = 3 same as 2 but using Wegstein acceleration. Default is COM CON = 1,1.

For columns with high compositional dependence of K-values, COM CON = 5, 1 is recommended. For use with APISOUR K-value option COM CON = 10, 2 is recommended. For use with APISOUR when NH₃, H₂S or CO₂ flow is high compared to water COM CON = 30, 3 is recommended. Also for an unconverged amine column, COM CON = 30, 3 should be considered.

DVS =

Enter the fractional change in vapor rates allowed when setting up column matrix. Default is 0.08, a range of 0.001 to 0.15 is recommended.

For columns with high vapor to liquid ratios, a DVS value can be calculated by dividing the minimum liquid rate by the average vapor rate, then dividing the answer by 2; for instance, if the liquid flowrate to the top were 1000 MOLE/HR, and the vapor flowrates were 10000 MOLE/HR:

$$DVS = 1000 / (2)(10000) = 0.05$$

DTS =

Enter the fractional change in tray temperature allowed when setting up column matrix. Default is 0.05, a range of 0.001 to 0.15 is recommended. The value of DTS should be about half the DVS value entered.

T SStep =

Enter the maximum temperature change to be used during column convergence. This number also represents the maximum percent change in the average column vapor rate allowed. Default is 150.

For a more stable column convergence, normally for columns displaying high vapor rate dependence on temperature (cryogenic demethanizers), a value of 50 is recommended.

Distillation: Super Convergence Technique

Enter the SUPer command to select the SUPer convergence technique. Enter any of the other commands to adjust the SUPer convergence control parameters. The default values are satisfactory for most runs and have been set to converge normal columns in the least amount of time. For nonideal columns consider adjusting the COM CON and DVS parameters. Do not use the T SStep command with the SUPer convergence technique. DTS is not normally needed with SUPer.

SUPer

Specifies the use of the SUPer convergence technique. Do not use with Absorber or LLE columns.

TOLerance =

Enter the maximum acceptable NORM for the column. The NORM for SUPer is defined as the square of the errors in the changes in the K-values and enthalpies plus the square of the errors for any component recovery specification. The default is TOL = 0.1 E-4.

For recycle loop calculations involving distillation columns where PROduct rate is not a specification, recycle loop convergence usually can be speeded up by changing the TOLerance to 0.1E-5.

MAXimum MATrices=

Enter the maximum number of matrix inversions for column solution. Default is 25.

Since the SUPer convergence technique is fast, the MAX MAT command normally is not used. A well-specified column may require four or five matrix inversions. Most columns will converge within 10 matrix inversions. The default number of matrix inversions is 25, which would take only about 50 percent longer than ten matrix inversions.

COMpositional CONvergence =

To stabilize compositional dependent K-values enter two numbers separated by commas. The first is the number of times

during initial column setup that K-values are recalculated in allowing for composition effects. The second number determines how many of these K-value recalculations are performed before the vapor rate profiles are recalculated. Default is COM CON = 5,2.

For columns with high compositional dependence of K-values, COM CON = 10, 2 is recommended. The value of the first number should never be greater than 20. The second number should be about half the first number. For K-value options that are typically used to model nonideal systems, such as MDEAK, APISOUR, WILson, RENon, UNIQUACK, and UNIFAC, COM CON = 10,2 is the default value.

DVS =

Enter the averaging factor to dampen oscillations between iterations during convergence. Default is 1. A range of 0.2 to 1 is recommended.

The K-value used in the calculation is figured as follows: $K_{\text{used}} = (1 - \text{DVS}) * K_{\text{old}} + \text{DVS} * K_{\text{new}}$

For compositional dependent columns, a DVS = 0.5 is recommended and will cause averaging of the K-values from one iteration to the next. A DVS as small as 0.2 can be used. Small values of DVS slow convergence, but convergence may not be possible otherwise.

MATrix

Enter this command to use SUPER with a MATrix technique. This is normally not required.

MAXimum DIMension =

Enter a value for the number of trays plus two when the MATRIX technique is used with SUPER and the number of trays exceeds 120.

Distillation: Super Plus Convergence Technique

Enter the SUPER PLUs command to select an alternative convergence technique. It is primarily a technique to improve convergence for a mixture of components with a wide range of boiling points or a solvent whose boiling point is significantly different than the rest of the mixture. The SUPER PLUs technique automatically adjusts the COM CON and DVS parameters to enhance convergence for a broad spectrum of applications. However, you can enter values for these parameters to override the automatic adjustment. The SUPER PLUs convergence parameters have the same meaning as those for SUPER and entered values have approximately the same effect. Do not use the DTS, T STEP, MATrix, or MAXimum DIMENSION commands with the SUPER PLUs convergence technique.

SUPER PLUs

Specifies the use of the SUPER PLUs convergence technique. Do not use with Absorber or LLE columns.

TOLerance =

Enter the maximum acceptable NORM for the column. The NORM for SUPER PLUs is defined as the square of the errors in the changes in the K-values and the enthalpies plus the square of the errors for any component recovery specification. The default is TOL = 0.1 E-4.

For recycle loop calculations involving distillation columns where PRODUCT rate is not a specification, recycle loop convergence can usually be speeded up by changing the TOLerance to 0.1 E-5.

MAXimum MATrices =

Enter the maximum matrix inversions for column solution. Default is 25.

Since the SUPER PLUs convergence technique is fast, the MAX MAT command normally is not used. A well-specified column may take four or five matrix inversions. Most columns will converge within 10 matrix inversions. The default number of matrix inversions is 25, which would take only about 50 percent longer than ten matrix inversions.

COMpositional CONvergence =

To stabilize compositional dependent K-values enter two numbers separated by commas. The first is the number of times, during initial column setup, that K-values are recalculated in allowing for composition effects. The second number determines how many of these K-value recalculations are performed before the vapor rate profile is recalculated. Default is COM CON = 5,2.

The SUPER PLUs technique automatically adjusts the second number to enhance convergence. To override this automatic adjustment, enter the second number with a negative value (for example: COM CON = 5,-2 will behave like COM CON = 5,2).

For columns with high compositional dependence of K-values, COM CON = 10, 2 is recommended. The value of the first number should never be greater than 20. The second number should be about one-third the first number. For K-value options that are typically used to model nonideal systems, such as MDEAK, APISOUR, WILson, RENon, UNIQUAC, and UNIFAC, COM CON = 10,2 is the default value.

DVS =

Enter the averaging factor to dampen K-value oscillations during convergence iterations. If the DVS command is not entered, then the SUPER PLUs technique automatically adjusts the DVS parameter to enhance column convergence. The default value starts at 1 and is adjusted continuously during the column calculation. A value in the range of 0.2 to 0.999 can be entered to override the automatic adjustment. If DVS is to be entered, see the recommendations given in the discussion of SUPER.

Distillation: Sum Rates Convergence Technique

SUM RATES is a two or three phase convergence method for Distillation Columns (condenser only, reboiler only, and when with both condenser & reboiler). SUM RATES also includes support for three phase liquid-liquid columns. This method can also support calculations when side draws, inter-coolers and tray heaters are present. Do not use this command with SUPER or SUPER PLUs convergence options.

Notes:

1. Top and Bottom Product purity & component flow rate specification items are not yet supported for condenser only, reboiler only and condenser/reboiler columns.
2. For liquid-liquid intercoolers the liquid intercooler will only draw the second liquid phase and the vapor intercooler will only draw first liquid phase.

Distillation Command Summary

Column Type

ABSorber
ABSorber with **RE**Boiler
PRESATurator
TEMperature of **CH**iller (T units) =
LLE
STRipper
STRipper with **TOTAL** condenser
PARTial fractionator
TOTAL fractionator

Required Column Description

TRAys =
TEMperature **TOP** guess (T units) =
TEMperature **BOT**om guess (T units) =
PREssure of **TOP**tray (p units) =
PREssure of **BOT** tray (p units) =
DELta pressure (P units) -
LOCation of **FEE**ds =
PROduct rate (molar Q/t units of **FRA**ction) =

Convergence Techniques

SUPER
SUPER PLUs
SUM RATES

Reflux Specifications

REFlux ratio =
REFlux **FLO**wrate (Q units/t units) =

Condenser and Reboiler Specifications

TEMperature of **COND**enser (T units) =
DUTy of condenser (H units/t units) =
TEMperature of **RE**Boiler (T units) =
REBoiler duty (H units/t units) =

Non-molar Product Rate Specifications

TOTAL PROduct **TOP** (Q units/t units) =
TOTAL PROduct **SIDE** n(Q units/t units) =
TOTAL PROduct **BOT**tom (Q units/t units) =

Side Draws

LOCation of **SIDE** draws =

Condenser

PREssure out of **COND**enser (P units) =
REFlux **GUE**ss =
TEMperature out total **COND**enser (T units) =
TEMperature **COND**enser **SUB**cooling (T units) =

Thermosiphon Reboiler Calculation

THErmosiphon vapor fraction =

Decant Water and Other Immiscible Components

DECanting **COM**ponent =
LOCation of **DEC**ants =
DECant **RAT**e guess (molar Q units/t units) =
DECant in **REF**lux =
IMMiscible =

Column Efficiency

EFFiciency of **COL**umn =
EFFiciency of **BASE** component **i** =

Tray Sizing

SPacing of **TR**Ays (L units) =
WEir **HE**ight (L units) =
WEir **LEN**gth (L units) =
DOWncomer **ARE**a (L2 units) =
GLitsch **SYS**tem factor =
GLitsch **PER**cent flood =
GLitsch **SW**age trays =
GLitsch **PAS**ses per tray per section =
GLitsch **SP**acing per tray per section (L units) =
GLitsch **DIA**meter per tray per section (L units) =
GLitsch **DOW**ncomer **ARE**a per tray per section (L2 units) =
GLitsch **WE**ir **HE**ight per tray per section (L units) =
GLitsch **VAL**ve **TY**pe =
GLitsch **VAL**ve **MAT**erial =
GLitsch **VAL**ve **TH**ickness (L units) =
GLitsch **VAL**ve **NUM**ber per ft2 =
GLitsch **DECK** thickness (L units) =
GLitsch **SW**age trays =

Calculation Options

CO2 FREeze
CONDensing **CUR**ve
REBoiler **CUR**ve
BUBble point =
DEW point =
LIQuid =
VAPor =
INTercooler **STR**eam **x** =
CONDenser **STR**eam =
CONDenser **SEP**arator **STR**eam =
REBoiler **STR**eam =
HEAter **STR**eam **i** =
TEMperature of **HEA**ting fluid (T units) =
TEMperature of **COO**ling fluid (T units) =

Thermodynamics Commands

HKEy =
KKEy =
DKEy =

Column Profiles

TEMperature **PRO**file guess (T units) =
VAPor **PRO**files (molar Q units/t units) =
REBoiler **VAP**or **GUE**ss (molar Q / t units) =
LIQuid **COM**position profile **i** =
PREssure **PRO**files (P Units) =
PREssure of **BOT**tom (P units) =
SAVE PROfiles
SAVE TEMperature profile

NO IMMiscible

Extractive (entrainer) Column Calculations

EXTRactive COMponent =

Tray Heaters and Coolers

LOCation of HEATers or coolers =

HEAT (H units/t units) =

LOCation of INTERcoolers (T units) =

TEMPerature out of INTERcoolers (T units) =

DUTy of INTERcoolers (H units/t units) =

DELta TEMperature of INTERcoolers (T units) =

DUTy of INTERcooler GUESS (H units/t units) =

TEMPerature of INTERcooler GUESS (T units) =

Print Options

SMithSIZing OFF

GLitsch SIZing OFF

PLOt OFF

PRInt SWItch =

LIGht KEY =

SAVe VAPor profile

SAVe LIQuid profile

SAVe MATrix

Regular Convergence Technique

TOLerance =

MAXimum MATrices =

COMpositional CONvergence =

DVS =

DTS =

T Step =

Super Convergence Technique

SUPER

TOLerance

MAXimum MATrices =

COMpositional CONvergence =

DVS =

MATrix

MAXimum DIMENsion =

Super Plus Convergence Technique

SUPER PLUS

TOLerance =

MAXimum MATrices =

COMpositional CONvergence =

DVS =

Product Composition Specifications

PURity in TOP (MOLar or MASS, RELative or ABSsolute) i =

PURity in BOTtom (VOLume, RELative) i =

PURity in SIDE draw n (MOLar or MASS, RELative or ABSsolute) i =

RECovery in TOP (MOLar or MASS - Q/t units, RELative or ABSsolute) i =

RECovery in BOTtom (GALSTP/HR) i =

RECovery in BOTtom (M3NTP/HR) i =

RECovery in SIDE draw n (MOLar or MASS - Q/t units, RELative or ABSsolute) i =

RATio in TOP (MOLar or MASS, RELative or ABSsolute) i,j =

RATio in BOTtom (MOLar or MASS, RELative or ABSsolute) i,j =

RATio in SIDE draw n (MOLar or MASS, RELative or ABSsolute) i,j =

Distillation Step-by-Step

Distillation STEP 1

Enter all the information at the right to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet stream(s)

DIS

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited number, in top-to-bottom order

Maximum of nine, in top-to-bottom order

Distillation STEP 2

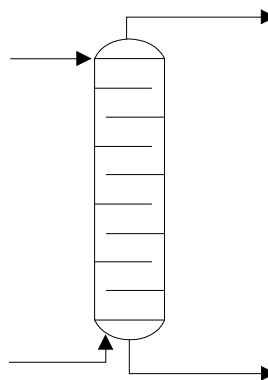
Select ONE column type from the main configurations.

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Optionally, specify presaturator for ABS and ABS REB column types. If no condenser and no reboiler, THEN select absorber column type.

Absorber column

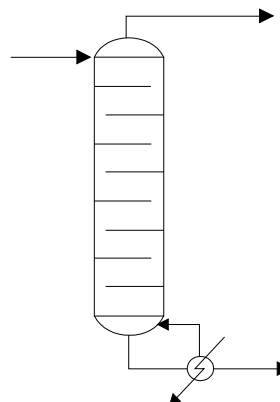
ABS



If no condenser but with a reboiler, THEN select absorber with reboiler

Absorber with reboiler column

ABS REB

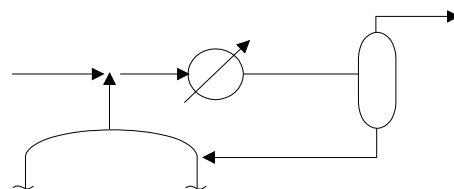


If ABS or ABS REB, optionally specify presaturator

Presaturator

Chiller temperature (required)

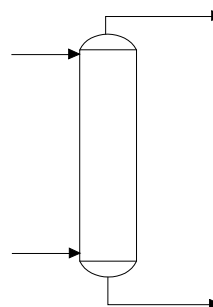
PRE SAT
TEM CHI (T units) =



If ABS with liquid feed to top and bottom tray

Liquid-Liquid Exchanger column

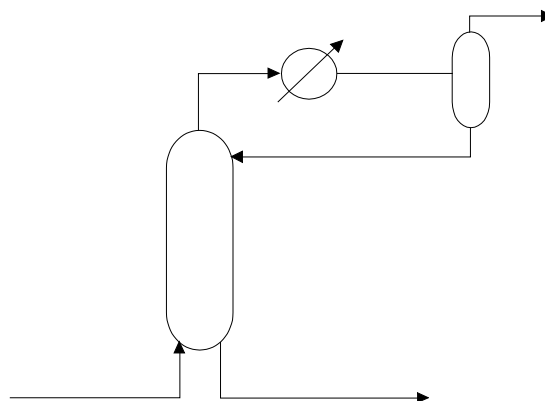
LLE



If a partial condenser but no reboiler, THEN select stripper column

Stripper Column

STR



If a total condenser but no reboiler, THEN select stripper with total condenser column.

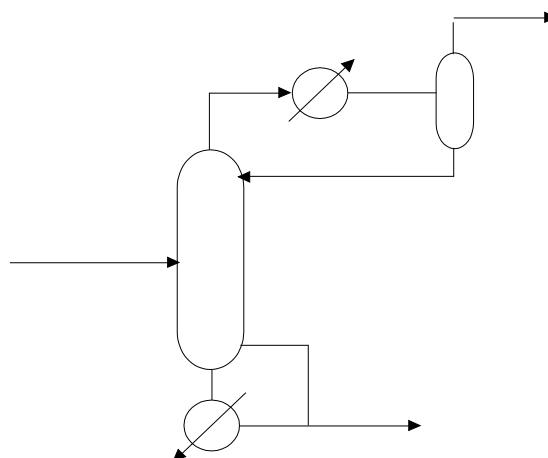
Total Condenser Column

STR TOT

If a partial condenser and a reboiler, THEN select partial fractionator column

Partial Fractionator Column

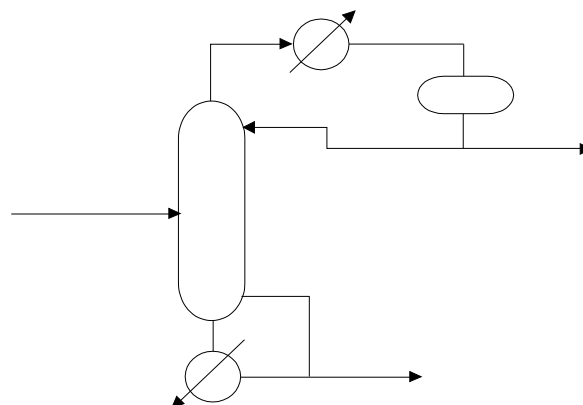
PAR



If a total condenser and a reboiler, THEN select total fractionator column

Total Fractionator Column

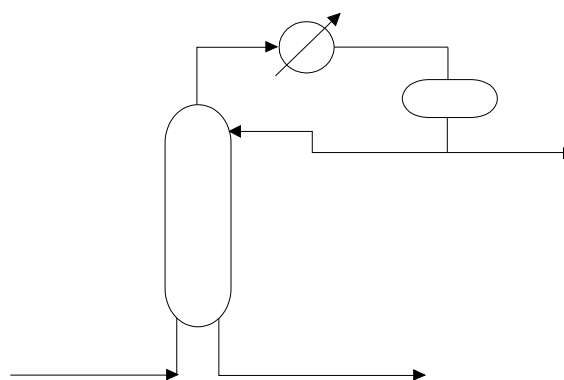
TOT



Distillation STEP 3

Enter the required column description.

Required column description (enter ALL of the following)



Number of theoretical trays (not including reboilers or condensers, top tray = 1)

Top product temperature guess (use top tray temperature if condenser temperature specified)

TRA =
TEM TOP (T units) =

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later)

Bottom product temperature guess

Top tray pressure

Column pressure drop (default is 0)

Feed tray locations (enter tray numbers separated by commas in top-to-bottom order)

Product molar flowrate guesses (or specification; enter molar flowrates for all products separated by commas in top-to-bottom order; enter zero for either top or bottom product rate)

TEM BOT (T units) =

PRE TOP (P units) =

DEL (P units) =

LOC FEE =

PRO (molar Q units/t units or **FRA**ction) =

Distillation STEP 4

Choose one of the four convergence techniques.

Regular, can only be selected by default below

Super convergence technique, can also be selected by default below

Super Plus convergence technique, cannot be selected by default

Sum Rates convergence technique, cannot be selected by default

SUP

SUP PLU

SUM RATES

Default selection criteria if no technique chosen

Four Convergence techniques are available: Regular, SUPer, SUPer PLUs and SUM RATES.

- Regular is always required if column type is either: ABS, ABS with PRESATurator, or ABS REB with PRESATurator. Regular is selected by default if TRAYS are 59 or less and all selected heat and material balance specifications are Regular (R) in table below.
- SUPer is selected by default if TRAYS are greater than 59 or at least ONE of the selected heat and material balance specifications is a SUPer (S) specification in the following table.

Regular (R) and SUPer (S) default specifications

Specification	ABS REB	PRESAT	STR	STR TOT	PAR	TOT
PRO	R	R	R	R	R	R
REF	-	-	R	R	R	R
REF FLO	-	-	S	S	S	S
TEM COM	-	-	R	-	R	-
DUT CON	-	-	R	R	S	S
TEM REB	R	R	-	-	S	S
REB	R	R	-	-	R	R
TOT PRO	S	-	S	S	S	S
PUR	S	-	S	S	S	S
REC	S	-	S	S	S	S
RAT	S	-	S	S	S	S
Inline FORTRAN	S	-	S	S	S	S

Distillation STEP 5

Select heat and material balance specification(s).

Choose the number of specifications required based on the column type

Column type	Number of specifications required
ABS	no specifications
ABS REB	1 specification
STR	1 specification
STR TOT	1 specification
PAR	2 specifications
TOT	2 specifications

Select specifications from the following 6 categories:

1. Molar product flowrate specification

Top or bottom product molar flowrate entered previously as guess with PRO = command in STEP 3. (The top or bottom guess is used as a specification only if the number of required specifications are not met with the commands below).

2. Reflux specifications (only ONE can be selected)

Molar reflux ratio

Reflux flowrate

REF =

REF FLO (molar, mass, or volume Q units/t units) =

3. Condenser and reboiler specifications (only ONE can be selected)

Temperature of condenser (specification for PAR and STR column types only)

Duty of condenser

Temperature of reboiler

TEM CON (T units) =

DUT CON (H/t units) =

TEM REB (T units) =

Reboiler duty

REB (H/t units) =

- 4. Product composition specifications** (Enter purity, recovery, or ratio specifications replacing “i” and “j” with DESIGN II component ID numbers. Units can be MOLar or MASSs and error can be RELative or ABSolute basis. MOLar and RELative options where they apply are defaults.)

Molar or mass fraction of component “i” in top product

PUR TOP (MOLar or MASSs, RELative or ABSolute) i =

Molar or mass fraction of component “i” in the nth side draw

PUR SID n (MOLar or MASSs, RELative or ABSolute) i =

Molar or mass fraction of component “i” in bottom product

PUR BOT (MOLar or MASSs, RELative or ABSolute) i =

Molar or mass flowrate of component “i” in top product

REC TOP (MOLar or MASSs - Q/t units, RELative or ABSolute) i =

Molar or mass flowrate of component “i” in the nth side draw

REC SID n (MOLar or MASSs - Q/t units, RELative or ABSolute) i =

Molar or mass flowrate of component “i” in bottom product

REC BOT (MOLar or MASSs - Q/t units, RELative or ABSolute) i =

Molar or mass ratio of components “i” & “j” in top product

RAT TOP (MOLar or MASSs, RELative or ABSolute) i,j =

Molar or mass ratio of components “i” & “j” in the nth side draw

RAT SID n (MOLar or MASSs, RELative or ABSolute) i,j =

Molar or mass ratio of components “i” & “j” in bottom product

RAT BOT (MOLar or MASSs, RELative or ABSolute) i,j =

- 5. Non-molar (mass or volume) product flowrate (Do not specify both top & bottom)**

Total vapor distillate flowrate

TOT PRO TOP (Q units/t units) =

Total side draw flowrate for nth side draw product

TOT PRO SID n (Q units/t units) =

Total bottom product flowrate

TOT PRO BOT (Q units/t units) =

- 6. Inline FORTRAN Specifications.** One or two specifications can be defined with Inline FORTRAN to replace purity or recovery specifications. See *Inline Fortran: Table 3. Distillation Function*.

Distillation STEP 6

Specify optional column description.

Side draw locations

Tray locations of unstripped side draws from top to bottom, separated by commas. Negative numbers indicate vapor draw

LOC SID =

Condenser Options

Pressure out of condenser (default is top tray pressure)

PRE CON (P units) =

Molar reflux guess

REF GUE =

Condenser temperature (for STR TOT and TOT column types only)

TEM CON (T units) =

or

Degrees subcooled (for STR TOT and TOT column types only)

TEM CON SUB (T units) =

Thermosiphon reboiler

Mole fraction that is vaporized of thermosiphon reboiler outlet stream (default is kettle reboiler)

THE =

Decant water or other immiscible component (use only DEC COM to decant from condenser alone, use DEC COM and LOC DEC to decant from trays as well as condenser)

Decant component ID number (for water, DEC COM = 62)

DEC COM =

Tray number(s) from which the component will be decanted (the condenser tray is tray zero), requires SUPer convergence command

LOC DEC =

Estimate total decant flowrate (optional)

DEC RAT =

Mole fraction of decant component in reflux (optional, program will calculate if not defined)

DEC REF =

Use ONE of the following commands to change

- immiscible component ID number (for water, IMM=62) default:

IMM =

- or, treat water as miscible

NO IMM

Extractive (entrainer) column

Identify extractive or entrainer component ID number for gasohol or extractive columns, requires SUPer

EXT COM =

Distillation STEP 7

Specify tray heaters and coolers.

Tray heaters and coolers (if present, enter BOTH commands). Enter values separated by commas in top-to-bottom order)

Tray number(s) on which the tray heaters and coolers are located

LOC HEA =

Duties for heaters and coolers (positive for heating, negative for cooling)

HEA (H units) =

Intercoolers (if present, enter only TWO commands) [enter LOC INT and only one of: TEM INT (optional-TEM INT GUE), DUT INT (optional-DUT INT GUE), DEL TEM INT, enter values separated by commas in top-to-bottom order]

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Tray numbers of intercooler draws (positive numbers are liquid draws, negative numbers are vapor draws, vapor draws require SUPER)
Intercooler return temperatures
Intercooler cooling duties (positive values), requires SUPER
Intercooler temperature drops (positive values), requires SUPER
Enter a guess for the heat added to or removed from each intercooler in top to bottom order
Enter an estimate for the intercooler return temperatures

LOC INT =

TEM INT (T units) =

DUT INT (H units/t units) =

DEL TEM INT (T units) =

DUT INT GUE (H units/t units) =

TEM INT GUE (T units) =

Distillation STEP 8

Column efficiency options. (All optional)

Efficiency of the Column

EFF COL =

Efficiency of the base (heavy key) component

EFF BAS i =

Select tray sizing options. **Smith-Dresser-Ohlswager** technique (All optional) (Enter all commands to replace 18 inch default setting height)

Spacing of trays

SPA TRA (L units) =

Weir height

WEI HEI (L units) =

Weir length

WEI LEN (L units) =

Downcomer area (default is 12% of empty column area)

DOW ARE (L2 units)=

Glitsch technique (All optional) (Enter GLI PER to calculate diameters or enter GLI DIA to calculate percent flood. Do not enter both GLI PER and GLI DIA)

System factor for foaming (one value, default is 1)

GLI SYS =

Percent of flood (one value, default is 80%)

GLI PER =

Number of tray passes (one value: 1,2, or 4 passes)

GLI PAS per tray per section =

Tray spacing(s) (default is 2 feet)

GLI SPA per tray per section (L units) =

Diameter(s) of trays

GLI DIA per tray per section (L units) =

Tray number(s) immediately below swage (for columns with more than one diameter or spacing)

GLI SWA =

Enter the total downcomer area per tray. Will be calculated, when not provided.

GLI DOW ARE per tray per section (L2 units) =

Enter the weir height to be used along with GLitsch SPACING in calculating the settling height. Default is 3 inch

GLI WEI HEI per tray per section (L units)=

Enter the valve type. Either 1 or 4 is available. Default is 1.

GLI VAL TYPE =

Enter the valve material. Default is carbon steel.

GLI VAL MAT =

Enter the valve thickness. Default is 0.06 inch.

GLI VAL THI (L units) =

Enter the number of valves per square foot. Default is 13.

GLI VAL NUMBER (1/L2 units) =

Enter the deck thickness. Default is 0.104 inch.

GLI DECK thickness (L units) =

Distillation STEP 9

Select calculation and print options.

CO2 FREEze

Check for CO2 freeze

CO2 FRE

Condenser and reboiler curves

Request condenser curve output

CON CUR

Request reboiler curve output

REB CUR

Feed phase (enter stream number(s) for feeds entering the column to force the following conditions)

Feed is bubble point liquid at tray pressure

BUB =

Feed is dew point vapor at tray pressure

DEW =

Calculate feed enthalpy as if all liquid

LIQ =

Calculate feed enthalpy as if all vapor

VAP =

Internal Streams

Columns with condenser (PAR, STR, TOT, STRTOT, PRESAT) where 'x' is a stream number assigned to the tray 1 vapor and 'y' is a stream number assigned to the product sent to the reflux accumulator

CON STR = x, -y

Columns with condensers (PAR, STR, TOT, STRTOT, PRESAT) where 'x' is a stream number assigned to the stream sent to the reflux accumulator and stream number 'y' is assigned to the stream exiting the separator (reflux) back to the tray 1 of the main column.

CON SEP STR = x, -y

Columns with kettle reboilers (PAR, TOT and ABS) where 'x' is a stream number assigned to the bottom tray liquid, 'y' is a stream number assigned to the vapor

REB STR = x, -y, -z

return and 'z' is a stream number assigned to the bottoms product

Columns with thermosiphon reboilers (THE command is present) where 'x' is a stream number assigned to the reboiler feed and 'y' is a stream number assigned to the reboiler return

REB STR = x, -y

For columns with side heaters. The side heater on Tray 'i+1', takes the liquid stream from tray 'i' and creates an internal stream number 'x'. Stream number 'y' is assigned to the exit stream from the side heater.

HEA STR i = x, -y

Columns with intercoolers (ABS, ABS REB, SR, STR TOT, PAR, and TOT) where 'i' is the tray number, 'x' is a stream number assigned to the intercooler feed and 'y' is a stream number assigned to the intercooler return

INT STR i = x, -y

NOTE: The stream numbers used for internal streams should not be connected to other external process equipment modules.

If thermo is different than global (GENeral section) THEN select

K-value option
Enthalpy option
Density option

KKE =
HKE =
DKE =

Tray sizing print options

Delete Smith-Dresser-Ohlswager calculation and output
Delete Glitsch calculation and output
No column sizing output (PRInt SWItch=0 also suppresses column sizing output)

SMI SIZ OFF
GLI SIZ OFF
COL SIZ OFF

Plotted output

Suppress all plotted output

PLO OFF

Identify light and heavy keys (enter component ID numbers for an additional plot)

Light key component ID
Heavy key component ID

LIG KEY =
HEA KEY =

Control column output

Print switch number (-2, -1, 0, 1, 2, 3) to control column output (default is 2)

PRI SWI =

Lost work (enter changes to GENeral section specifications)

Heating fluid (utility side) temperature (default is 250 F)
Cooling fluid (utility side) temperature (default is 70.3 F)

TEM HEA (T units) =
TEM COO (T units) =

Distillation STEP 10

Enter optional column profiles. Enter tray profile commands as needed. For profiles enter guesses for each TRAY separated by commas in top-to-bottom order. Zeros entered between values indicates straight line interpolation for trays listed as zeros.

Temperature guess for each tray
Vapor rate guess for each tray
Guess for the vapor rate leaving the reboiler. Enter one value
Liquid mol fraction for component "i" for each tray. Regular convergence technique only not SUPer or SUPer PLUs.
Desired pressure for each tray
Pressure of the bottom product
Save column profiles between process recycle iterations
Save column matrix between process recycle iterations. Regular convergence technique only not SUPer or SUPer PLUs
Save column temperature profiles only between process recycle iterations
Save column vapor profile only between process recycle iterations
Save column liquid profile only between process recycle iterations

TEM PRO (T units) =
VAP PRO (molar Q units/t units) =
REB VAP GUE (molar Q/t units) =
LIQ COM i =

PRE PRO (P units) =
PRE BOT (P units) =
SAV PRO
SAV MAT

SAV TEM
SAV VAP
SAV LIQ

Distillation STEP 11

Enter optional convergence control parameters for one of three techniques.

Regular convergence technique.

Allowable error in tray heat and material balance (default is 0.1E-4)
Maximum number of matrix inversions (default is 6)
To stabilize compositional K-values enter two numbers separated by commas; first is the number of K-value iterations during each internal iteration; second is the iteration option: 1 for no iteration, 2 to iterate, 3 to use Wegstein acceleration. (default is 1,1)
Fractional change in vapor rates allowed when setting up column matrix. (range is 0.001 to 0.15, default is 0.08)
Fractional change in tray temperature allowed when setting up column matrix (range is 0.001 to 0.15, default is 0.05)

TOL =
MAX MAT =
COM CON =

DVS =

DTS =

Chapter 11

Maximum temperature change and maximum percent change in vapor rate per iteration (default is 150)

TST =

Super Convergence Technique

Specifies the use of the SUPer convergence technique

Allowable error in tray heat and material balance (default is 0.1E-4)

Maximum number of matrix inversions (default is 25)

To stabilize compositional K-values enter two numbers separated by commas; first is the number of initial K-value iterations; second is the number of times these iterations are performed before initial profiles are generated (1 to 5). (default is 5.2)

Averaging factor for K-values (range is 0.2 to 1.0, default is 1.0)

Use SUPer with a MATrix technique

If above MATrix technique used with SUPer and number of trays exceeds 120, enter a value which is the number of trays +2

SUP

TOL =

MAX MAT =

COM CON =

DVS =

MAT

MAX DIMEN =

SUPer PLUs convergence technique

Specifies the use of the SUPer PLUs convergence technique

Allowable error in tray heat and material balance (default is 0.1E-4)

Maximum number of matrix inversions (default is 25)

To stabilize compositional K-values enter two numbers separated by commas; first is the number of initial K-value iterations; second is the number of times these iterations are performed before initial profiles are generated (1 to 5) (default is 5.2)

Averaging factor for K-values (range is 0.2 to 1.0, default is 1.0)

SUP PLU

TOL =

MAX MAT =

COM CON =

DVS =

Distillation: Troubleshooting Column Calculations

When the column does not converge a message is printed just before the column profiles. The following general step-by-step review of the output can be used in locating possible problems.

1. Review Echo Print Of Input

Check the input commands for the column in the "ECHO PRINT OF INPUT DATA" to make sure all data was entered correctly. Check for any typing errors. Verify that all keyword entries are spelled or abbreviated correctly. Verify that the number zero is not being used for the letter "O" or vice versa. Verify that all input commands appear in their appropriate section, i.e., GENeral, DIStillation, etc. Did you code either the top or bottom rate as zero in the required PROduct rate command? Did you enter the correct number of heat and material specifications based on the selected column type?

2. Review Column Input Summary And Feed Flash

Product rates - Check the top or bottom product rate that was calculated by the program to achieve material balance. An incorrectly calculated rate may reveal an error in the LOC FEEd or the PROduct rate command. For columns in recycle loops, it is always advisable to enter the smaller of the top and bottom product rates (guess or specification). Calculations will stop if PROduct rates exceed feed rates to the column.

Required information - Check that all required column information has been entered, i.e., column pressures, temperature guesses, number of trays, heater or cooler and side draw information and specification selections.

Feed location, phase and K-values - Check the feed flash output for tray location, feed vapor and liquid separation, and whether the K-values look reasonable. If the feed location is incorrect, the desired specifications may be impossible. For instance, if the vapor feed is not entering below the bottom tray for an ABSorber type column, the column calculations will stop. The vapor fraction and liquid fraction composition of a feed can cause a specification to be impossible. For instance, if only 30 LBMOL/HR of n-pentane is in the liquid portion of the feed to a top feed stabilizer (column with no reflux) then a recovery in the bottom of 30 LBMOL/HR or greater would be impossible.

Strange looking K-values can mean the thermodynamic option you are using is inappropriate or that the feed pressure is wrong (near the critical pressure).

The accuracy of the distillation column results varies directly with the applicability of the K-values and enthalpy techniques for your particular system. A complete list of K-value, enthalpy and other thermophysical property options can be found in *Thermodynamics Section*.

Consider specification and convergence changes - If your input information seems correct, consider changing to an easier heat and material balance specification to get converged results. These results can then be used to improve temperature and molar flowrate guesses for the more difficult case. Also consider changing to another convergence technique choosing from the three available: regular, SUPer, or SUPer PLUs boiling range. Finally, if the system K-values are compositionally dependent (UNIFACK, WILson, RENon, UNIQUACK, APISOUR, MDEAK, SELEXOL K, and some systems with other K-values), it may be necessary to adjust the convergence control parameters: COM CON, DVS, etc.

3. Review The Column Update Summary

Initial NORM - During the iterations to obtain convergence, the NORM is printed to signify how close the column is to convergence at each step. The initial NORM value printed is very important since it reflects the accuracy of the input guesses. If the number is greater than 100, the initial column profiles generated from the input guesses are bad. Review the guesses and check the temperature guesses by running dew or bubble points on your desired products.

NORM slowly improving - If the NORM is reasonable, but is improving very slowly, the specifications are either very difficult or impossible based on the feed composition and location, theoretical trays and column pressure.

NORM improvement stops toward end - Columns separating only two components or columns separating components with large boiling point differences (greater than 50 F) display a slow improvement in the NORM just before the iterations stop. The product rates for these columns are very limited in range because only two components are being separated or because of the easy separation of components with large boiling point differences. These columns can normally be converged by adjusting the product rate based on the product compositions from the first run. For example, in a particular problem, the bottoms product rate was specified as 1775 LBMOL/HR for a column that did not converge. The feed and products calculated by the DISTillation module are:

Feed	Overhead		Bottoms
n-C4	40	38	.000003
i-C4	30	29	.000003
n-C5	15	15	.0003
i-C5	10	10	.0003
C6	25	25	.04
Lean oil	1775	3.0	1775
Total	1895	120	1775

Because of the large boiling point difference between C6 and the lean oil, and because 3.0 LBMOL/HR of the lean oil appears in the overhead, the column can only approach convergence. A material balance on the light components shows their flowrates had to be reduced to allow the total product rate of 120 LBMOL/HR to be met since 3.0 LBMOL/HR of lean oil also went overhead. Changing the product rate to 1772, allowing the loss of 3.0 LBMOL/HR of lean oil, results in a converged run. Be as accurate as possible when back calculating correct product rates to make sure the next run converges. Be careful in balance calculations in the regular convergence technique, since component material balance is assured only at convergence.

4. Review Column Profiles

Temperature profiles - Large temperature fluctuations or no change in temperature for several trays can be signs of convergence problems. If temperatures are fluctuating, they may require stabilizing by using the TStep and DTS commands described in *Distillation: Regular Convergence Technique*.

If the temperatures are the same for several trays, the trays are normally inefficient and could be removed until the column is converged. If necessary, the trays can then be added back and a TEMperature PROfile (extrapolated from the converged run) entered to promote convergence.

An unconverged column using the SUPer distillation technique may have a temperature profile with large inversions. No useful information can be extracted from this profile except that either TEM TOP and TEM BOT and/or PRO are inconsistent with the product composition specification.

Rather than trying to guess new values for TEM TOP, TEM BOT and PRO, try one of these approaches:

- Use the COMponent SPLitter (or SHORtcut fractionator for PARTial and TOTal columns) and specify the desired overhead product recoveries (flowrate or fractional basis) for each component. Specify TEM TOP DEW or BUB (vapor or liquid product, respectively) and TEM BOT BUB. This calculation will give you product rates and top and bottom product temperatures.

- Run the rigorous column calculation using PRO (and REFlux ratio, if two specifications are required) and the regular convergence technique. This calculation should converge easily. Enter temperature profiles from this calculation for the SUPer run. You can also review product information to see how far a given product rate is from matching your desired product composition specifications.

Vapor and liquid profiles - Vapor and liquid profiles should be checked for small flowrates which may indicate that the vapor or liquid rate on a tray is nearing zero during convergence. Changes in PROduct rate, LOCation of FEEds, or REFlux ratio may solve these problems. Also, if the liquid rate is much smaller than the vapor rate, a smaller value for DVS may be required in regular convergence technique (see *Distillation: Regular Convergence Technique*).

For columns with multiple feeds (particularly cryogenic demethanizers or deethanizers), check to be sure that the second feed is not revaporizing the liquid portion of the top feed. If this is occurring, consider lowering the temperature of the second feed.

5. **Review Products** - Check individual component material balance when the NORM stops improving. Make sure components are going to the correct product. If a component is to go to the overhead but is going to the bottoms, your column pressure or specifications may need to be adjusted.
6. **Review Condenser And Reboiler Duties** - Make sure the condenser and reboiler duties look reasonable. For instance, if there is too much heat in the feed, the reboiler duty may become negative.
7. **Review Enthalpies For Vapor And Liquid** - Check enthalpy profiles. Pay particular attention to trays where there is very little difference in vapor and liquid enthalpies, particularly if column pressure is within 50-100 PSIA of the product critical pressure. It may be necessary to switch to the standard enthalpy technique, then use the temperature profile from a converged run when you use the more accurate enthalpy technique.
8. **Review Tray-by-tray** - Vapor and liquid compositions should be studied from tray-to-tray to determine if the changes are reasonable. If the changes are erratic, a COM CON command may be useful. The feed tray compositions could also show an incorrect feed location. For the regular convergence technique (not SUPer or SUPer PLUs), the sum of the vapor compositions should be checked to see where the column is having problems meeting tray balances. Problems around the feed tray can possibly be solved by moving the feed or changing the feed temperature. Problems at the top or bottom normally result from incorrect product rate or purity specifications. Problems in between feeds and product trays may be from instabilities and the DVS or DTS commands may be needed.

Distillation Examples

There are many sample flowsheets in “Chapter 17: Distillation Column Samples - c:\designii\samples\equipmnt\distill” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 12: Divider

The DIVider module divides a stream into two to six other streams of the same composition, temperature, and pressure. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed stream pressure.

The DIVider module is often used with the CONTroller to divert part of a stream to optimize heat exchange or component recoveries. If you enter only the fraction or flowrate to go to the first output stream, the DIVider module automatically places the remainder in the second output stream. A CONTroller module can then be used to control the DIVider by varying a single fraction or flowrate. This technique works only when a DIVider has two output streams. If the DIVider you want to control has more than two outputs, break it into two DIViders, so that the one you control will have only two output streams (be sure your output streams are coded in the correct order).

Divider Command Details

FLOW RATE (FRAction or Q/t units) =

Enter the fractions or the flowrates to be allocated to each output stream. The fractions or flowrates are separated by commas and must be coded in the same order as their outlet stream numbers are coded on the equipment module command. FRAction is the default option.

If the feed to the DIVider has insufficient flow to satisfy the Q/t units value(s) specified with FLOW RATE, the program will respond as follows:

1. For two outlet streams, all feed to the DIVider will be placed in the first outlet stream.
2. For three or more outlet streams, as many of the specifications as possible will be satisfied. Any remaining specifications which cannot be satisfied because of insufficient flow will be ignored. Any remaining flow will be divided equally among the remaining outlet streams.

Divider Command Summary

Major Specifications

FLOW RATE (FRAction or Q/t units) =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Divider Step by Step

Divider STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

DIV

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

Two to six

Divider STEP 2

Enter the fractions or flowrates to be allocated to each output stream, separated by commas. Enter how input streams are to be divided.

Output flowrates (default is FRActions)

FLO RAT (FRA or Q/t units) =

IF thermo is different from global (GENeral section) options THEN select:

K-value option

Enthalpy option

Density option

KKE =

HKE =

DKE =

Divider Examples

There are several sample flowsheets in "Chapter 18: Divider Samples - c:\designii\samples\equipmnt\divider" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 13: Double Pipe Exchanger

The DOuble PIpe exchanger module can be used to calculate counter current heat exchange between two streams. The module calculates the heat and material balance from known input stream information and the specification to be met.

At this time, the Double Pipe Exchanger uses the Heat Exchanger unit module for it's calculations. In the future, the Double Pipe Heat Exchanger will get it's own unit module calculations and rating.

Double Pipe Exchanger Features

Stream Order

The HEAt EXChanger module always applies your specification to the first stream in and out. The pressure drop command contains information for both the first and second outlet streams. The order in which the streams are coded determines the stream to which your specifications will be applied. For instance:

```
HEAt EXChange 1 = E101, 3, 1, -4, -2, TEMperature OUT = 70
```

In the above example, to specify the temperature of stream 4 to be .70 F, you must code stream 4 as the first output stream.

Assumed Input

The HEAt EXChanger module assumes that all the properties of the inlet streams are known. Properties such as temperature, pressure, enthalpy, and component flowrates must be known in order to calculate the heat exchange. If one of the inlet streams is not known at the time the module is calculated, the calculation is not performed, and the known properties of the inlet stream are transferred to its outlet.

Duties

To specify heat addition to a stream, you use the DUTy command with a positive value for the heat addition. A negative value indicates heat removed. The output for the exchanger will report a positive Q for heat added to the first inlet stream or a negative Q for heat removed from the first inlet stream.

Dew or Bubble Point Feeds to the Exchanger

If a feed to a HEAt EXChanger module is to be at its dew point or bubble point, special care should be taken to insure that this condition is achieved by the program and is not just an estimate on your part. For example, if the feed is a pure component or narrow boiling mixture at bubble point, guessing at the temperature and pressure can result in the wrong phase, because the dew point temperature will not be much different than the bubble point. If your guess is off by even a degree, the feed could be half vapor. To make sure your bubble or dew point feeds are at the right temperature and have the proper phase, put them through a HEAt EXChanger module and specify the bubble or dew point to be calculated. Remember, this needs to be done only for feed streams and not intermediate streams that will be calculated by the program.

Double Pipe Exchanger Command Details

Double Pipe Exchanger: Counter-Current Commands

This exchanger simulates two process streams exchanging heat with each other, usually a heat recycle situation with one of the streams coming from downstream in the process.

For counter-current exchangers, remember to keep your input and output streams in the correct order, make sure your streams are coded so the specification is applied to the correct stream, and review your problem to see if the heat recycle can be removed.

If a SIMple exchanger is specified, the surface area and overall heat transfer coefficient of the exchanger should also be specified. If not, the area per shell will default to 100 FT² and the overall heat transfer coefficient will default to 50 BTU/HR/FT²/ F

Output

All outlet stream properties are calculated. The duty, area per shell, and corrected log mean temperature difference are reported. This is an iterative process which would require more execution time than a TEMperature OUT or DUTy specification.

Specifications Available (enter only one of the following)

SIMple exchanger

AREa and given U are used to calculate the temperatures out. Specify the AREa and U commands with this option

AREa (L units) =

Enter the area per shell for the SIMple exchanger specification. Default is 100 FT² (9.29 M²).

and

Chapter 13

U (U units) =

Enter the overall heat transfer coefficient. Default is 50 BTU/HR/FT²/ F (0.2839 KJ/SEC/M²/ K).

TEMperature **OUT** Shell Side (T units) =

Enter desired temperature of the stream coded as the first outlet stream. This is for shell side outlet stream.

TEMperature **OUT TUB**e Side (T units) =

Enter desired temperature of the tube side outlet stream.

DUTy (H units/t units) =

Enter the desired enthalpy change (- for cooling, + for heating) of the stream coded as the first input stream.

Shell Side **TEM**perature **OUT** is **BUB**ble point

Sets temperature of stream coded as the first outlet stream to the bubble point. This is for shell side outlet stream.

Shell Side **TEM**perature **OUT** is **DEW** point

Sets temperature of stream coded as the first outlet to the dew point. This is for shell side outlet stream.

TEMperature **AP**proach (T units) =

Absolute temperature difference between stream coded as the first outlet stream and stream coded as the second input stream (must be greater than 2 F). Note that the order of streams is with respect to the shell and tube side streams on flowsheet.

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 **GEN**eral section (please see [Calculation Options: Heat Exchanger Temperature Crossover](#)).

Shell Side **DEL**ta **TEM**perature (T units) =

Enter the desired change in temperature from inlet to outlet. +ve value indicates heating; -ve value indicates cooling. This specification is for the shell side outlet stream.

Double Pipe Exchanger: Counter-Current Optional Commands

NOTE: If you enter a value for **AREa** which is inconsistent with the area calculated from exchanger geometry your specified **AREa** will be used.

Double Pipe Exchanger Optional Command Details

Double Pipe Exchanger: Basic Optional Commands

DELta pressure (P units) =

Enter pressure drop through the exchanger. For two inlet streams enter the pressure drop for the stream coded first, a comma, then the pressure drop for the second stream. Default is zero.

U (U units) =

Enter the overall heat transfer coefficient. Default is 50 BTU/HR/FT²/F (0.2839 KJ/SEC/M²/ K).

AREa (L² units) =

Enter the area per shell for the **SIM**ple exchanger specification or the **WAT**er **COO**led exchanger option. Default is 100 FT² (9.29 M²).

Double Pipe Exchanger: Additional Output Commands

The **GEN**eral section also has **HEATING CUR**ve and **COOLING CUR**ve commands which can be used on any stream in the flowsheet. Heating or cooling curve information, shown below, can be obtained for a heat exchanger by specifying the following command types:

COMMAND 1:

CURve **INC**rements =

Enter the number of increments for heating curves.

Example:

```
HEAT EXCHANGER IN CONDENSING CURVE MODE
NUMBER OF TEMPERATURE INCREMENTS ON STREAM 1 = 4
EQUIPMENT NUMBER = 1
FOLLOWING CALCULATIONS BASED ON END POINT OF HEAT EXCHANGER
TOTAL HEAT TRANSFERRED FROM STREAM 1, BTU/HR .38010E 07 AREA = 2764.7 FT2 CORRECTED LOG MEAN TEMP. =
27.50 DEG F
MOL. WT. STREAM 1 = 20.50 MOL. WT. STREAM 2 = 17.01
FOLLOWING CALCULATIONS ARE FOR HEAT EXCHANGER DIVIDED INTO INCREMENTS
      STREAM 1          STREAM 2  ENTHALPY
INC    TEMP  VAPOR    TEMP  VAPOR    CHANGE    AREA    LMTD
NO     DEG F  FRAC    DEG F  FRAC    BTU/HR    FT2     DEG F
1      27.50  0.00    27.50  0.00    1000.00    1000    1.000
2      27.50  0.00    27.50  0.00    1000.00    1000    1.000
3      27.50  0.00    27.50  0.00    1000.00    1000    1.000
4      27.50  0.00    27.50  0.00    1000.00    1000    1.000
5      27.50  0.00    27.50  0.00    1000.00    1000    1.000
6      27.50  0.00    27.50  0.00    1000.00    1000    1.000
7      27.50  0.00    27.50  0.00    1000.00    1000    1.000
8      27.50  0.00    27.50  0.00    1000.00    1000    1.000
9      27.50  0.00    27.50  0.00    1000.00    1000    1.000
10     27.50  0.00    27.50  0.00    1000.00    1000    1.000
11     27.50  0.00    27.50  0.00    1000.00    1000    1.000
12     27.50  0.00    27.50  0.00    1000.00    1000    1.000
13     27.50  0.00    27.50  0.00    1000.00    1000    1.000
14     27.50  0.00    27.50  0.00    1000.00    1000    1.000
15     27.50  0.00    27.50  0.00    1000.00    1000    1.000
16     27.50  0.00    27.50  0.00    1000.00    1000    1.000
17     27.50  0.00    27.50  0.00    1000.00    1000    1.000
18     27.50  0.00    27.50  0.00    1000.00    1000    1.000
19     27.50  0.00    27.50  0.00    1000.00    1000    1.000
20     27.50  0.00    27.50  0.00    1000.00    1000    1.000
21     27.50  0.00    27.50  0.00    1000.00    1000    1.000
22     27.50  0.00    27.50  0.00    1000.00    1000    1.000
23     27.50  0.00    27.50  0.00    1000.00    1000    1.000
24     27.50  0.00    27.50  0.00    1000.00    1000    1.000
25     27.50  0.00    27.50  0.00    1000.00    1000    1.000
26     27.50  0.00    27.50  0.00    1000.00    1000    1.000
27     27.50  0.00    27.50  0.00    1000.00    1000    1.000
28     27.50  0.00    27.50  0.00    1000.00    1000    1.000
29     27.50  0.00    27.50  0.00    1000.00    1000    1.000
30     27.50  0.00    27.50  0.00    1000.00    1000    1.000
31     27.50  0.00    27.50  0.00    1000.00    1000    1.000
32     27.50  0.00    27.50  0.00    1000.00    1000    1.000
33     27.50  0.00    27.50  0.00    1000.00    1000    1.000
34     27.50  0.00    27.50  0.00    1000.00    1000    1.000
35     27.50  0.00    27.50  0.00    1000.00    1000    1.000
36     27.50  0.00    27.50  0.00    1000.00    1000    1.000
37     27.50  0.00    27.50  0.00    1000.00    1000    1.000
38     27.50  0.00    27.50  0.00    1000.00    1000    1.000
39     27.50  0.00    27.50  0.00    1000.00    1000    1.000
40     27.50  0.00    27.50  0.00    1000.00    1000    1.000
41     27.50  0.00    27.50  0.00    1000.00    1000    1.000
42     27.50  0.00    27.50  0.00    1000.00    1000    1.000
43     27.50  0.00    27.50  0.00    1000.00    1000    1.000
44     27.50  0.00    27.50  0.00    1000.00    1000    1.000
45     27.50  0.00    27.50  0.00    1000.00    1000    1.000
46     27.50  0.00    27.50  0.00    1000.00    1000    1.000
47     27.50  0.00    27.50  0.00    1000.00    1000    1.000
48     27.50  0.00    27.50  0.00    1000.00    1000    1.000
49     27.50  0.00    27.50  0.00    1000.00    1000    1.000
50     27.50  0.00    27.50  0.00    1000.00    1000    1.000
51     27.50  0.00    27.50  0.00    1000.00    1000    1.000
52     27.50  0.00    27.50  0.00    1000.00    1000    1.000
53     27.50  0.00    27.50  0.00    1000.00    1000    1.000
54     27.50  0.00    27.50  0.00    1000.00    1000    1.000
55     27.50  0.00    27.50  0.00    1000.00    1000    1.000
56     27.50  0.00    27.50  0.00    1000.00    1000    1.000
57     27.50  0.00    27.50  0.00    1000.00    1000    1.000
58     27.50  0.00    27.50  0.00    1000.00    1000    1.000
59     27.50  0.00    27.50  0.00    1000.00    1000    1.000
60     27.50  0.00    27.50  0.00    1000.00    1000    1.000
61     27.50  0.00    27.50  0.00    1000.00    1000    1.000
62     27.50  0.00    27.50  0.00    1000.00    1000    1.000
63     27.50  0.00    27.50  0.00    1000.00    1000    1.000
64     27.50  0.00    27.50  0.00    1000.00    1000    1.000
65     27.50  0.00    27.50  0.00    1000.00    1000    1.000
66     27.50  0.00    27.50  0.00    1000.00    1000    1.000
67     27.50  0.00    27.50  0.00    1000.00    1000    1.000
68     27.50  0.00    27.50  0.00    1000.00    1000    1.000
69     27.50  0.00    27.50  0.00    1000.00    1000    1.000
70     27.50  0.00    27.50  0.00    1000.00    1000    1.000
71     27.50  0.00    27.50  0.00    1000.00    1000    1.000
72     27.50  0.00    27.50  0.00    1000.00    1000    1.000
73     27.50  0.00    27.50  0.00    1000.00    1000    1.000
74     27.50  0.00    27.50  0.00    1000.00    1000    1.000
75     27.50  0.00    27.50  0.00    1000.00    1000    1.000
76     27.50  0.00    27.50  0.00    1000.00    1000    1.000
77     27.50  0.00    27.50  0.00    1000.00    1000    1.000
78     27.50  0.00    27.50  0.00    1000.00    1000    1.000
79     27.50  0.00    27.50  0.00    1000.00    1000    1.000
80     27.50  0.00    27.50  0.00    1000.00    1000    1.000
81     27.50  0.00    27.50  0.00    1000.00    1000    1.000
82     27.50  0.00    27.50  0.00    1000.00    1000    1.000
83     27.50  0.00    27.50  0.00    1000.00    1000    1.000
84     27.50  0.00    27.50  0.00    1000.00    1000    1.000
85     27.50  0.00    27.50  0.00    1000.00    1000    1.000
86     27.50  0.00    27.50  0.00    1000.00    1000    1.000
87     27.50  0.00    27.50  0.00    1000.00    1000    1.000
88     27.50  0.00    27.50  0.00    1000.00    1000    1.000
89     27.50  0.00    27.50  0.00    1000.00    1000    1.000
90     27.50  0.00    27.50  0.00    1000.00    1000    1.000
91     27.50  0.00    27.50  0.00    1000.00    1000    1.000
92     27.50  0.00    27.50  0.00    1000.00    1000    1.000
93     27.50  0.00    27.50  0.00    1000.00    1000    1.000
94     27.50  0.00    27.50  0.00    1000.00    1000    1.000
95     27.50  0.00    27.50  0.00    1000.00    1000    1.000
96     27.50  0.00    27.50  0.00    1000.00    1000    1.000
97     27.50  0.00    27.50  0.00    1000.00    1000    1.000
98     27.50  0.00    27.50  0.00    1000.00    1000    1.000
99     27.50  0.00    27.50  0.00    1000.00    1000    1.000
100    27.50  0.00    27.50  0.00    1000.00    1000    1.000
```


0	-58.6	.6559	-127.9	.9971	.00000	0.0	0.0
1	-17.7	.8452	-56.1	1.0000	.12683E07	485.0	52.3
2	23.2	.9578	9.2	1.0000	.10662E07	883.0	24.2
3	64.1	.9996	60.0	1.0000	.83240E06	2073	8.0
4	105.0	1.0000	98.2	1.0000	.63411E07	2393	5.3

TOTAL AREA FOR 4 DIVISIONS IN THIS HXER = 5833.8 FT²

TOTAL HEAT TRANSFERRED = .39010+07 BTU/HR

Heat exchanger curves should be done as a separate run since the curve information requires a significant additional amount of time. By running heat exchanger curves in a separate run, you can be sure your process design is correct before spending time in final design information.

NOTE: The geometry of the exchanger for CUR INC output is based on one shell, one tube pass, one shell pass, regardless of the geometry commands entered for the heat exchanger. Stream 1 refers to the first inlet stream and stream 2 is the second inlet (tubewise).

COMMAND 2:

Q-T

Enter this command to have duty versus temperature curves plotted for heat exchangers.

The Q-T table and plot are useful tools for evaluating exchanger design. These curves are based on end-point temperature results. You can quickly determine the minimum temperature approach or locate regions with unrealistically high U x A or temperature crossovers. In addition, bubble points and dew points are marked when vaporization or condensation occurs for either hot or cold streams.

To get this additional report, add the command: **Q-T**

This command can be used in conjunction with HEAt EXChanger RATing.

NOTE: Use of the CURve INCrements command is not allowed with the Q-T command.

When using the **Q-T** command, the following print option may be useful.

COMMAND 3:

MINimum TEMperature APProach (T units) =

Used only with the Q-T command. Enter a minimum temperature of approach value. The first point where the approach temperature falls below this value will be marked with the label MN in the Q-T tabular output. Default is 10 F.

Sample output for the Q-T print option can be found in the LNG Exchanger Example 6 - *LNG Exchanger: Q-T Diagram*.

COMMAND 4:

TEMperature of EXChange (T units) =

Enter value for exchange temperature for the utility side of the exchanger (for single stream exchangers only). Default temperatures are 250 F for heating fluids, 70.3 F for cooling fluids. This command is used only in conjunction with the LOST work command which is entered in the GENeral section.

Double Pipe Exchanger: Thermodynamic Commands

Use these commands to specify options for the module only when they are different than the system thermodynamics specified in the GENeral commands. Options are given in Thermodynamics Section.

HKEY =

Enter symbolic name of enthalpy option. (e.g. **HKE = GRA**)

KKEY =

Enter symbolic name of K-value option. (e.g. **KKE = ESSOK**)

DKEY =

Enter symbolic name of density option. (e.g. **DKE = IDEALD**)

LIQUID DKEY =

Enter symbolic name for liquid density option.(e.g. **LIQUID DKEY = PEND**)

VSVKEY =

Enter symbolic name for vapor viscosity. (e.g. **VSVKEY = DEAN**)

VSLKEY =

Enter symbolic name for liquid viscosity. (e.g. **VSLKEY = API**)

THVKEY =

Enter symbolic name for vapor thermal conductivity. (e.g. **THVKEY = NBS81**)

THLKEY =

Enter symbolic name for liquid thermal conductivity. (e.g. **THLKEY = TEMA**)

STKEY =

Enter symbolic name for surface tension. (e.g. **STKEY = API**)

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The commands above specify the thermodynamics for shell side streams of counter-current (two-stream) exchangers. To specify different thermodynamics for the tubeside stream only, the following commands may be used.

HKEy 2 =

Enter symbolic name of enthalpy option for tubeside stream. (e.g. **HKE 2= GRA**)

KKEy 2 =

Enter symbolic name of K-value option for tubeside stream. (e.g. **KKE 2= ESSOK**)

DKEy 2 =

Enter symbolic name of density option for tubeside stream. (e.g. **DKE 2= IDEALD**)

LIQuid DKEY 2 =

Enter symbolic name for liquid density option.(e.g. **LIQuid DKEY 2 = PEND**)

VSVKEY 2 =

Enter symbolic name for vapor viscosity for tube side stream.. (e.g. **VSVKEY 2 = DEAN**)

VSLKEY 2 =

Enter symbolic name for liquid viscosity for tube side stream.. (e.g. **VSLKEY 2 = API**)

Double Pipe Exchanger Command Summary

Counter-Current Heat Exchangers Commands

SIMple exchanger

AREa (L2 units) =

TEMperature **APP**roach (T units) =

TEMperature **OUT** Shell Side (T units) =

TEMperature **OUT TUB**e Side (T units) =

DUTy (H units/t units) =

Shell Side **TEM**perature **OUT** is **BUB**ble point

Shell Side **TEM**perature **OUT** is **DEW** point

Shell Side **DEL**ta **TEM**perature (T units) =

Counter-Current Exchanger Optional Commands

U (U units) =

Additional Output Commands

CURve **INC**rements =

Q-T

MIN TEM APP (T units) =

Thermo for tubeside stream only

HKEy 2 =

KKEy 2 =

DKEy 2 =

Water Immiscibility

IMM = 62

NO IMM

Optional Commands

TEMperature of **EX**Change (T units) =

CURve **INC**rements =

DELta pressure (P units) =

U (U units) =

AREa (L2 unit) =

Thermo option for shellside and tubeside streams (two & single-stream exchanger)

HKEy =

KKEy =

DKEy =

LIQUID DKEY =

VSVKEY =

VSLKEY =

THVKEY =

THLKEY =

STKEY =

Thermo for tubeside stream only (two-stream exchanger only)

HKEy 2 =

KKEy 2 =

DKEy 2 =

LIQuid DKEY 2 =

VSVKEY 2 =

VSLKEY 2 =

THVKEY 2 =

THLKEY 2 =

STKEY 2 =

Double Pipe Exchanger Step by Step

Double Pipe Exchanger STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet stream(s)

DOU PIP

Assigned equipment flowsheet number

User choice - up to 16 characters

One or two

One or two - must match number of inlet streams

NOTE: The 1st inlet stream coded becomes 1st outlet stream coded and the 2nd inlet stream coded becomes the 2nd outlet stream coded.

Double Pipe Exchanger STEP 2

Choose a heat exchanger type. Select ONE of the following heat exchanger types.

- Counter-current; code with two inlet streams and two outlet streams
- first inlet stream coded will be shell side inlet

Double Pipe Exchanger STEP 3

Enter the required specifications and desired options for the selected heat exchanger type.

Counter-current exchanger (enter ONE of the following)

IF simple exchanger enter **ALL** of the following specifications

Simple exchanger

Heat transfer surface area per shell (stream outlet temperature is calculated from specified AREa and U; default is 100 FT²)

Overall heat transfer coefficient default is 50 BTU/HR/FT²/ F

Absolute temperature difference between stream coded as the first outlet stream and stream coded as the second input stream (must be greater than 2 F)

Temperature of stream coded as the first outlet stream (will correspond to the stream coded as the first inlet stream). This is for shell side outlet stream.

Temperature out of tube side

Enthalpy change (- for cooling, + for heating) of the stream coded as the first inlet stream
Set temperature of stream coded as the first outlet stream to the bubble point. This is for shell side outlet stream.

Set temperature of stream coded as the first outlet stream to the dew point. This is for shell side outlet stream.

Temperature change from inlet to outlet (+ value indicates heating; - value indicates cooling). This is for shell side outlet stream.

SIM

ARE (L units) =

U (U units) =

TEM APP (T units) =

TEM OUT (T units) =

TEM OUT TUB (T units) =

DUT (H units/t units) =

TEM OUT BUB

TEM OUT DEW

DEL TEM (T units) =

Double Pipe Exchanger STEP 4

Choose any of the optional heat exchanger specifications below.

Select any of the following options.

Pressure drop through the exchanger (for two inlet streams enter the pressure drops for the first and second streams separated by commas; default is zero)

Overall heat transfer coefficient (if U and AREa are not required commands, the AREa is calculated as $AREa = Q/U \cdot LMTD$); default is 50 BTU/HR/FT²/ F)

Heat transfer surface area per shell (default is 100 FT²)

DEL (P units) =

U (U units) =

ARE (L2 units) =

Double Pipe Exchanger STEP 5

Choose any of the additional options below. Additional output information (select ONE of the following).

Number of increments for heating/cooling curves, not allowed if the Q-T command is used (default is no curve)

Duty-temperature curve (default is no curve)

Minimum approach temperature (marks tabular output with the label "MN" at point of specified minimum approach)

CUR INC =

Q-T

MIN TEM APP (T units) =

Select ANY of the following options

Value for exchange temperature for the utility side of the exchanger (only used for single stream exchanger; default temperatures are 250 F for heating fluids, 70.3 F for cooling fluids)

TEM EXC (T units) =

This command is used only in conjunction with the LOST work command which is entered in the GENeral section.

If thermo is different from global (GENeral section) options THEN select the commands below. If specified, they will apply to shellside stream.

K-value option

Enthalpy option

Density option

Enter symbolic name for vapor viscosity.

Enter symbolic name for liquid viscosity.

Enter symbolic name for vapor thermal conductivity.

Enter symbolic name for liquid thermal conductivity.

Enter symbolic name for surface tension.

KKE =

HKE =

DKE =

VSVKEY =

VSLKEY =

THVKEY =

THLKEY =

STKEY =

To specify different thermo for tubeside stream only (counter-current only) select

K-value option for tubeside stream

Enthalpy option for tubeside stream

Density option for tubeside stream

KKE2 =

HKE2 =

DKE2 =

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Enter symbolic name for vapor viscosity for tube side stream.
Enter symbolic name for liquid viscosity for tube side stream.
Enter symbolic name for vapor thermal conductivity for tube side stream.
Enter symbolic name for liquid thermal conductivity for tube side stream.
Enter symbolic name for surface tension for tube side stream.

VSVKEY 2 =
VSLKEY 2 =
THVKEY 2 =
THLKEY 2 =
STKEY 2 =

Double Pipe Exchanger Examples

There are several sample flowsheets in “Chapter 25: Double Pipe Exchanger Samples -
c:\designii\samples\equipment\doublepipe” of the DESIGN II for Windows Tutorial and Samples Guide.

Double Pipe Exchanger References

1. Kakac, Sadik; Liu, Hongtan; Heat Exchangers: Selecton, Rating and Thermal Design, 2nd Edition, Department of Mechanical Engineering, University of Miami, Coral Gables, Florida

Chapter 14: Equilibrium Reactor

This generalized equilibrium reactor module calculates gas-phase reactions of multi-component systems. Chemical equilibrium can be calculated isothermally or adiabatically. Isothermal calculations are the default. This reactor module is not restricted to a specific type of reaction. Heat and entropy of formation data at 25C are required for all components. This data is available automatically for the first 98 components in the *Database Components*. See the Command Details for information on entering this data for other components. You can enter product constraints or stoichiometric coefficients for reactions occurring at conditions away from equilibrium such that extent of reaction or temperature of approach specifications can be used. You can use either the global reaction commands or the specific reaction commands to specify the products approach to equilibrium. If you do not enter any reaction commands, DESIGN II will automatically redistribute all atomic species among the specified molecular species to achieve the most thermodynamically stable molecular compositions. Since these are gas-phase reactions, one of the following equation of state techniques should be used:

APISOAVEK

LKPK

BWRK

PENK

BWRSK

RKK

Equilibrium Reactor Command Details

Equilibrium Reactor: Reaction Type

ADiabatic

Enter this command to have the calculation performed adiabatically (constant enthalpy). Default calculation is isothermal (constant temperature).

Equilibrium Reactor: Reaction Definition Commands

In this equilibrium reactor DESIGN II will redistribute all atomic species among the specified molecular species to achieve the most thermodynamically stable molecular compositions. The only required information for a reaction at equilibrium is the heat and entropy of formation data (please see details below to include this data under Specify...Component Data...Reaction Properties). The Equilibrium Reactor Optional Commands are used to enter general reaction information. The optional GUEssed product and INERt commands have the effect of speeding up the calculations. The PROduct constraint command sets the maximum allowable amount of component i in the product.

Reaction Approaching Equilibrium

You can specify the products approach to equilibrium in one of two ways: either GLOBAL or SPECIFIC. GLOBAL and SPECIFIC reaction commands **cannot** be mixed and they should be used individually.

GLOBAL REACTION COMMANDS

(enter one of the following two)

PROduct constraint (molar Q units/t units) i

Enter the flow of component i in the product stream, where i is the component ID number. This sets the amount of component i wanted in the product.

OR

TEMperature of APProach (T units) =

Enter the approach to equilibrium temperature for all reactions in this module.

SPECIFIC REACTION COMMANDS

These commands are used to enter specific information about an individual reaction. To use either the EXTent of reaction or TEMperature approach for REAction commands, you must first enter a Reaction j command. This command is of the form

$$Rj = (a1*r1 + a2*r2 + = b1*p1 + b2*p2 +)$$

where

a1,a2 are the stoichiometric coefficients for the reactants,

r1,r2 are the component ID numbers for the reactants,

b1,b2 are the stoichiometric coefficients for the products,

p1,p2 are the component ID numbers for the products,

j is the reaction number.

The stoichiometric coefficients are entered on a molar basis. Fractions are allowed.

For the following reaction,

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you would enter the following Reaction command:

$$\text{R1} = (1 \cdot 2 + 1 \cdot 62 = 1 \cdot 48 + 3 \cdot 1)$$

EXTent of reaction (molar Q/t units) **j** =

Enter the extent of reaction for reaction j, where j is the reaction number.

OR

TEMperature approach for **REA**ction (T units) **j** =

Enter the approach to equilibrium temperature for reaction j, where j is the reaction number.

NOTES:

1. Although reactions are described with stoichiometric coefficients on a molar basis, the reactions are not necessarily equimolar. Reactions will always be in mass balance. Having entered the Rj command, enter one of the following two commands
2. For specific adiabatic reactions using equilibrium reactor, please use negligible amount of CO₂ (1E-05) in the feed stream and specify CO₂ as an inert substance using INert=49 command.
3. All individual reactions should be numbered and defined in ascending order (ex.R1, R2, R3 and NOT R2,R1, R3 or R3,R2,R1). A total of 24 reactions are allowed per reactor module.

Defining Heat and Entropy of Formation Data

Reactions may be defined as continuing to equilibrium or approaching equilibrium. For either of the above two cases, heat of formation and entropy of formation data must be supplied. For components with ID numbers from 1 -98 these data are stored on the pure component data base and automatically accessed. For components with ID numbers greater than 98 you must supply the data at 25C using the following commands in the GENeral section of the input file (or under Specify...Component Data...Reaction Properties of the flowsheet file):

HEAt of **FOR**mation (H units/molar Q units) **i** =

Enter the heat of formation where i is the component ID number.

ENTropy of **FOR**mation(H units/molar Q units/T units) **i** =

Enter the entropy of formation where i is the component ID number. The allowable units are as follows:

BTU/LBMOL/R (default)

KCAL/KGMOL/K

CAL/GMOL/K

J/GMOL/K

KJ/KGMOL/K

For example,

GENeral

COMponents = 2,49,48,62,1021

ENTropy of **FOR**mation (BTU/LBMOL/R) 1021 = -30.9907

HEAt of **FOR**mation (BTU/LBMOL) 1021 = -86544,

Equilibrium Reactor Optional Commands

The following commands are optional. They may be used independent of the type of reaction defined.

GUEssed products (Q units/t units) =

Enter product flow guesses for each component in the same order as they appear in the COMponents list. As an alternative for entering a product guess, omit this command and enter a FLOWrate in the GENeral section for the product stream from the EQUilibrium REActor.

INert =

Enter the ID numbers of the components which are not involved in the reaction(s). These components are inert; they do not participate in the reactions, but do participate in the enthalpy balances.

MAXimum **ITE**rations =

Sets the number of iterations performed. Default is 30.

HEAt (H units/ t units) in =

Enter an optional heat duty specification to be transferred to the equilibrium reactor.

Equilibrium Reactor Command Summary

Reactor Type

Default is isothermal

ADIabatic

Heat and Entropy of Formation

Only required if component ID is >98; put in GENERAL section of input file.

HEAt of **FOR**mation (H units/molar Q units) **i** =

ENTropy of **FOR**mation (H/molar Q/T units) **i** =

Optional commands

GUEssed products (Q units/t units) =

INErt =

MAXimum **ITE**rations =

Reactions Approaching Equilibrium

Global reaction

PROduct constraint (molar Q units/t units) **i** =

or

TEMperature of **APP**roach (T units) =

or

Specific reaction

Rj = (a1*r1 + a2*.. = b1*p1 + b2*p2 + ..)

and one of the following

EXTent of reaction (molar Q/t units) **j** =

Equilibrium Reactor Step by Step

Equilibrium Reactor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

EQU REA

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

One

NOTE: The **EQU**ilibrium **REA**ctor allows only vapor phase calculations.

Equilibrium Reactor STEP 2

Supply heat and entropy of formation data for components with ID numbers >98. Ensure heat and entropy of formation data is available.

For any reaction defined in this module, the heat and entropy of formation for each component must be available. The DESIGN II data base contains this data for components with ID numbers from 1 through 98. For components with ID numbers greater than 98, enter the data with the following two commands in the GENERAL section of the input file:

Heat of formation for component "i", where "i" is the component ID number **HEA FOR** (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** =

NOTE: The allowable units for ENT FOR are as follows:

BTU/LBMOL/R (default)

KCAL/KGMOL/K

KJ/KGMOL/K

CAL/GMOL/K

J/GMOL/K

Equilibrium Reactor STEP 3

Choose a reactor type. Default is isothermal

Adiabatic calculation (constant enthalpy)

ADI

Equilibrium Reactor STEP 4

Choose whether the reaction is at equilibrium OR approaching equilibrium. Define reaction as occurring at equilibrium or approaching equilibrium.

Reaction occurring at equilibrium

If an equilibrium reaction calculation is desired, no additional specifications are required. The only information required is the heat and entropy of formation data at 25 C for all components involved in the reaction.

OR

Reaction approaching equilibrium (use either GLOBAL or SPECIFIC reaction commands)

GLOBAL reaction commands (choose one of the following two)

Flow of component "i" in the product stream, where "i" is the component ID number (sets the maximum amount of component "i" allowed in the product)

approach to equilibrium temperature for all reactions

PRO (molar Q units/t units) **i** =

TEM APP (T units) =

SPECIFIC reaction commands

First, specify information about an individual reaction. Multiple reactions are allowed.

The form of the expression is

Rj = (a1*r1 a2*r2 + .. = b1*p1 + b2*p2 + ..)

a1,a2

stoichiometric coefficients for the reactants

r1,r2

component ID numbers for the reactants

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b1,b2 stoichiometric coefficients for the products
p1,p2 component ID numbers for the products
j reaction number

Next, enter ONE of the following commands per defined reaction Rj.

Extent of reaction “j”, where “j” is the reaction number (can only be used in conjunction with a Reaction “j” command) **EXT** (molar Q/t units) j =

Approach to equilibrium temperature for reaction “j”, where “j” is the reaction number (can only be used in conjunction with a Reaction “j” command) **TEM REA** (T units) j =

NOTE: Use of either the global or specific technique for defining a reaction away from equilibrium still requires heat and entropy of formation data for the components.

Enter any of the optional commands listed below.

Product flow guesses for each component in the same order as they appear in the COMponents list **GUE** (molar Q units/t units) =

ID numbers of the inert components which are not involved in the reaction (s) **INE** =

Set the number of iterations (default is 30) **MAX ITE** =

Equilibrium Reactor Examples

There are several sample flowsheets in “Chapter 19: Equilibrium Reactor Samples - c:\designii\samples\equipmnt\equireac” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 15: Expander

The EXPander module performs an isentropic expansion of liquid, vapor, or two-phase streams to a specified outlet pressure; actual work is then calculated from the ideal work and the user-supplied efficiency, and the final temperature and phase distribution is calculated using the actual work. The CALculated WORK is stored as a positive number. An example of how the CALculated WORK from an EXPander can be used to drive a compressor is presented in the CONTroller module.

An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure before expansion. Either one or two output streams can be coded. If two output streams are coded, the vapor is placed in the first output and liquid in the second output.

NOTE: If the input streams are liquid, only one output stream should be coded.

Expander Command Details

PREssure OUT (P units) =

Enter desired discharge pressure. Default is one-half of suction pressure.

PREssure DELta (P units) =

Enter desired pressure change or delta pressure. Default is one-half of suction pressure.

EFFiciency = *fraction*

Enter the efficiency of the EXPander. Default is 0.72.

TEMperature OUT (T units) =

Enter desired temperature. Efficiency will be calculated.

Expander Command Summary

Specification Commands

PREssure OUT (P units) =

PREssure DELta (P units) =

EFFiciency = *fraction*

TEMperature OUT (T units) =

(Efficiency will be calculated)

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Expander Step by Step

Expander STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

EXP

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

One or two; if two, 1st is vapor, 2nd is liquid

Expander STEP 2

Enter the required specifications listed below. Performance specifications (BOTH are required).

Discharge pressure

Pressure change or delta pressure

Temperature Out. (*Efficiency will be calculated*).

PRE OUT (P units) =

PREssure DELta (P units) =

TEM OUT (T units) =

Choose any of the optional specifications listed below.

IF thermo is different from global (GENeral section) options THEN select:

K-value option

Enthalpy option

Density option

KKE =

HKE =

DKE =

Expander Examples

There are several sample flowsheets in “Chapter 20: Expander Samples - c:\designii\samples\equipmnt\expander” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 16: Expander Compressor

The EXPander COMpressor module is a utility module that passes or uses the calculated work by the expander to the compressor as the maximum available work. The expander part of the module is similar to the stand alone EXPander module that performs an isentropic expansion of liquid, vapor, or two-phase streams to a specified outlet pressure; actual work is then calculated from the ideal work and the user-supplied efficiency. The stored CALculated WORK is a positive number and will be automatically used by the compressor portion of the module as the maximum available work.

Only two input streams and two output streams can be assigned for the combined module by the user. If the isentropic calculation is specified, a rigorous mixed-phase calculation is performed. If the isentropic calculation is not specified, the liquid is compressed as if it were a vapor. If the compressor feed vapor fraction is less than 0.9, the module shifts to a pump calculation.

Expander Compressor Command Details

PREssure OUT EXPander (P units) =

Enter desired discharge pressure for the expander compressor module. Default is one-half of suction pressure.

ISEntropic **EFF**iciency **EXP**ander = fraction

Enter the isentropic efficiency of the expander portion of the EXPander COMpressor module. Default is 0.72.

ISEntropic **EFF**iciency **COM**pressor = fraction

Enter the isentropic efficiency of the compressor/ pump portion of the EXPander COMpressor module. Default is 0.65.

To simulate a centrifugal compressor when you know the Cp/Cv ratio and polytropic efficiency, the CALculate POLytropic coefficient COMpressor command can be used. If you have manufacturer's curves for an existing centrifugal compressor, you should consider using the POLytropic compressor module. The temperature for the POLytropic COEfficient of COMpressor case is calculated from the enthalpy difference due to the pressure change and work added to the system. Please note that polytropic coefficient cannot be calculated or provided for a pump.

For **Polytropic pump** calculation the following can be used.

POLytropic **EFF**iciency of **COM**pressor = *fraction*

Enter polytropic efficiency for a pump. Default is 0.72.

For **Polytropic compressor** calculation either ONE of the following combinations can be used.

CALculate **POL**ytropic coefficient **COM**pressor

This is the default calculation option.

and

POLytropic **EFF**iciency of **COM**pressor = *fraction*

Enter polytropic efficiency of compressor. Default is 0.72.

(OR)

POLytropic **COE**fficient of **COM**pressor =

Enter the polytropic coefficient $[(n-1)/n]$. Default for the dimensionless coefficient is 0.22 (with $n = 1.282$). Allowed only for compressor and not for a pump.

and

POLytropic **EFF**iciency of **COM**pressor = *fraction*

Enter polytropic efficiency of compressor. Default is 0.72.

Expander Compressor Optional Command Details

COUpling **EFF**iciency = *fraction*

Enter the coupling efficiency on the work produced by expander to be used by compressor. Default is 1.0.

COUpling **LOS**s (Power Units) =

Enter the coupling loss due to lost mechanical work by the compressor. Default is 0.0 HP.

Expander Compressor Command Summary

Specification Commands

PREssure **OUT EXP**ander (P units) =
ISEntropic **EFF**iciency **EXP**ander = *fraction*
ISEntropic **EFF**iciency **COM**pressor = *fraction*
CALculate **POL**ytropic coefficient **COM**pressor
POLytropic **EFF**iciency of **COM**pressor = *fraction*
POLytropic **COE**fficient of **COM**pressor = *fraction*

Optional Commands

COUpling **EFF**iciency = *fraction*
COUpling **LOS**s (Power Units) =

Thermodynamics Commands

HKEy =
KKEy =
DKEy =

Expander Compressor Step by Step

Expander Compressor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier	EXP COM
Equipment number	Assigned equipment flowsheet number
Equipment name	User choice - up to 16 characters
Inlet stream	Two in number
Outlet streams	Two in number

Expander Compressor STEP 2

Enter the required specifications listed below. Performance specifications (BOTH are required).

Discharge pressure	PRE ssure OUT EXP ander (P units) =
Expander isentropic efficiency (default is 0.72)	ISE ntropic EFF iciency EXP ander = <i>fraction</i>
Compressor or Pump isentropic efficiency (default is 0.65)	ISE ntropic EFF iciency COM pressor = <i>fraction</i>
Enter polytropic efficiency of pump. Default is 0.72.	POL ytropic EFF iciency of COM pressor = <i>fraction</i>
Default calculation option (not available for pump).	CAL culate POL ytropic coefficient COM pressor
and	
Enter polytropic efficiency of compressor. Default is 0.72.	POL ytropic EFF iciency of COM pressor = <i>fraction</i>
Enter the polytropic coefficient [(n-1)/n]. Default for the dimensionless coefficient is 0.22 (with n = 1.282).	POL ytropic COE fficient of COM pressor =
and	
Enter polytropic efficiency of compressor/pump. Default is 0.72	POL ytropic EFF iciency of COM pressor = <i>fraction</i>

Choose any of the optional specifications listed below.

Coupling Efficiency	COU pling EFF iciency = <i>fraction</i>
Coupling Loss in power	COU pling LOS s (Power Units) =

IF thermo is different from global (GENeral section) options THEN select:

K-value option	KKE =
Enthalpy option	HKE =
Density option	DKE =

Expander Compressor: Example

There are several sample flowsheets in "Chapter 21: Expander Samples - c:\designii\samples\equipment\expcom" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 17: Fired Heater

The fired heater module calculates the fuel consumption and actual heater duty when a process stream is heated to a given temperature. The heating value of the fuel and the heater efficiency can be specified along with the rated duty of the heater. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure. Either one or two output streams can be coded. If two output streams are coded, the vapor is placed in the first output and liquid in the second output.

Fired Heater Command Details

TEMperature **OUT** (T units) =

Enter the desired temperature of the process stream.

RATing of **HEA**ter (H/t units) =

Enter the rated duty to be used as the heating limit. Outlet temperature will be reduced if this limit is exceeded. Default is 1 x 10⁹ BTU/HR (2.93 x10⁵ KJ/SEC).

Fired Heater Optional Commands

DELta pressure (P units) =

Enter the pressure drop.

EFFiciency = *fraction*

Enter the fuel efficiency. Default is 0.75.

HEAting **VAL**ue of **FUE**l (H/molar or vapor volume Q units) =

Enter the heating value of the fuel. Default is 900 BTU/SCF.

TEMperature of **EX**change (T units) =

Enter the exchange temperature for the LOST WORK analysis. Default is 250F.

Fired Heater Command Summary

Required Commands

TEMperature **OUT** (T units) =

RATing of **HEA**ter (H/t units) =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Required Commands

TEMperature **OUT** (T units) =

RATing of **HEA**ter (H/t units) =

Optional Commands

DELta pressure (P units) =

EFFiciency =

HEAting **VAL**ue of **FUE**l (H/molar or vapor volume Q units) =

TEMperature of **EX**change (T units) =

Fired Heater Step by Step

Fired Heater STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

FIR

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

One or two; if two, 1st is vapor, 2nd is liquid

Fired Heater STEP 2

Enter the required fired heater specifications listed below. Enter the outlet temperature and fired heater rating.

Fired heater outlet temperature

Fired heater rated maximum duty (default is 10E9 BTU/HR)

TEM OUT (t UNITS) =

RAT HEA(H/t units) =

Choose any of the optional specifications listed below. If heater options are desired, THEN select any of the following

Pressure drop (default is 0 PSI)

Fuel efficiency (default is 0.75)

Fuel heating value(default is 900 BTU/SCF)

DEL (P units) =

EFF = fraction

HEA VAL FUE (H/molar or vapor volume Q units) =

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IF LOST work option, THEN select the following

Exchange temperature for lost work (default is 250 F) **TEM EXC** (T units) =

IF thermo is different from global (GENERAL section) options THEN select:

K-value option **KKE** =

Enthalpy option **HKE** =

Density option **DKE** =

Fired Heater Example

There are several sample flowsheets in "Chapter 22: Fired Heater Samples - c:\designii\samples\equipmnt\firedhea" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 18: Flash

The FLash module can separate the vapor and liquid phases of a single two-phase stream. An essentially unlimited number of inlet streams can be coded; they will be adiabatically mixed at the lowest feed pressure. Three outlet streams may be coded if IMMiscible = 62 is specified in the GENeral section, or you have specified a K-value option which automatically treats water as immiscible. The first outlet stream will contain the vapor phase; the second outlet stream will contain the hydrocarbon liquid phase plus soluble water; and the third outlet stream will contain "free" water plus soluble hydrocarbons. For the three-phase hydrocarbon-water system, you can also specify entrainment in the two liquid phases.

Flash Features

The FLash module can separate the vapor and liquid phases of a single two-phase stream. An essentially unlimited number of inlet streams can be coded; they will be adiabatically mixed at the lowest feed pressure. Three outlet streams may be coded if IMMiscible = 62 is specified in the GENeral section, or you have specified a K-value option which automatically treats water as immiscible. The first outlet stream will contain the vapor phase; the second outlet stream will contain the hydrocarbon liquid phase plus soluble water; and the third outlet stream will contain "free" water plus soluble hydrocarbons. For the three-phase hydrocarbon-water system, you can also specify entrainment in the two liquid phases.

A heat loss or gain can be specified for adiabatic calculations. Isentropic and an additional isothermal calculation method (as used in the multiple flash module) may also be specified. The VALve module should be used when pressure change is desired or when streams are to be mixed before flashing. If the HEAt change is not specified, the phase separation will be isothermal.

You can request sizing calculations for any of the single stage separators on your flowsheet by using a few extra commands in your input. These results are intended for preliminary design work only and should not be used for detailed vessel design to A.S.M.E. code requirements (Reference 5). Simplifying assumptions have been made to facilitate preliminary sizing. The program can size any vertical or horizontal liquid-vapor separators such as flash drums, reflux drums, accumulators, water knockout drums and inlet gas or compressor inlet separators.

Different types of separators can be sized in a single run using sizing commands available on either the FLash or VALve module. Physical properties of the vapor and liquid phases are obtained automatically from the program. These properties correspond to the vessel outlet conditions.

An appropriate selection of K-value and density options should be made to obtain best results. DESIGN II gives you a wide choice of sizing specifications and uses reasonable default values if you do not specify any. Vessel diameter, length and thickness are calculated, and total weight of steel is estimated using a percentage allowance for supports and fittings. A scaled sketch is given for vertical vessels indicating the relative dimensions, liquid level and nozzle positions.

An unlimited number of input streams may be coded. When no specification is given and more than one input stream is coded, DESIGN II performs an adiabatic flash at the lowest feed pressure. However, if only one feed stream is coded and no specification is given, then DESIGN II performs an isothermal flash at the feed temperature and pressure.

Flash Command Details

Flash: Calculation Options

There are two calculation methods for an isothermal flash. The FLash method (default) performs an isothermal flash at the inlet conditions. Isothermal flashes may also be performed at a specified temperature and pressure, using the MULTiple FLash module algorithm.

ISOthermal flash

Specifies an isothermal calculation using the MULTiple FLash algorithm rather than the default FLash calculation.

There are two calculation methods for an adiabatic flash. The FLash algorithm performs an adiabatic flash at the inlet conditions with a specified addition of heat using the HEAt command. The MULTiple FLash algorithm performs an adiabatic flash with specified heat addition, and temperature or pressure. This method is obtained by using the ADIabatic, DELta, HEAt, TEMperature OUT, and PREssure OUT commands. If neither TEMperature OUT nor PREssure OUT is specified, the flash will be performed using the lowest inlet pressure of the stream among the multiple inlet streams.

ADIabatic flash

Specifies the MULTiple FLash adiabatic (constant enthalpy) algorithm.

DELta pressure (P units)=

Enter this command to specify the pressure drop across the flash vessel.

HEAt change (H units/t units) =

Enter the heat change (negative for loss). Use alone for the FLash algorithm or with ADIabatic for the MULTiple FLash algorithm.

ISEntropic

Specifies an isentropic calculation.

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TEMPerature from **FEE**d

Specifies the temperature from feed stream.

PREssure from **FEE**d

Specifies the pressure from feed stream.

BUBble point

Requests calculation of bubble point temperature or pressure. Default is temperature.

BUBble point **TEM**perature

Requests calculation of bubble point temperature.

BUBble point **PRE**ssure

Requests calculation of bubble point pressure.

DEW point

Requests calculation of dew point temperature or pressure. Default is temperature.

DEW point **TEM**perature

Requests calculation of dew point temperature.

DEW point **PRE**ssure

Requests calculation of dew point pressure.

DEW WATER

Requests calculation of water dew point temperature or pressure (default is temperature). IMM=62 must be specified in the GENeral section.

DEW WATER TEMperature

Requests calculation of water dew point temperature. IMM=62 must be specified in the GENeral section.

DEW WATER PREssure

Requests calculation of water dew point pressure. IMM=62 must be specified in the GENeral section.

LIQuid **FRA**ction (**MOL**ar/**MA**SSs) =

Enter the fraction of hydrocarbon liquid desired in the outlet stream. Units are MOLar or MASSs. Default is MOLar.

VAPor

Forces the flow to go to vapor at the specified temperature and pressure regardless of the actual vapor-liquid distribution.

LIQuid

Forces the flow to go to liquid at the specified temperature and pressure regardless of the actual vapor-liquid distribution.

Flash: Outlet Pressure And Temperature Specifications

The FLash methods for isothermal and adiabatic flashes do not allow outlet stream specification. The flash is performed at the inlet conditions. The MULTiple FLash algorithm for isothermal flashes allows both PREssure OUT and TEMperature OUT specification. Otherwise, DESIGN II will use the inlet temperature and pressure as needed. For the MULTiple FLash algorithms for ADIabatic, HEAt change, ISEntropic, BUBble point, DEW point, DEW WATER, and LIQuid FRAction, either PREssure OUT or TEMperature OUT specification is required. If both are specified, PREssure OUT will be treated as the specification and the temperature will be treated as an initial guess.

PREssure **OUT** (P units) =

Enter the outlet pressure for the flash.

TEMperature **OUT** (T units) =

Enter the outlet temperature for the flash.

Flash: Lost Work Analysis

TEMperature of **EX**change (T units) =

Enter the exchange temperature for the fluid providing the heating (cooling) in the HEA command. Default temperatures are 250F for heating and 70.3 F for cooling. This command is only applicable to the LOST WORK analysis.

Flash: Non-Equilibrium Separations

When three outlet streams have been coded for the FLash module, and IMM=62 has been specified in the GENeral section, you can use the following commands to specify a non-equilibrium separation:

WATER ENTained In **OIL** (units) =

Enter fraction for water entrained in oil.

OIL ENTained in **WATER** (units) =

Enter fraction for oil entrained in water

Where the units option refers to MOLar fraction, VOLume fraction or MASs fraction.

NOTE: Where three outlet streams are specified, there are two options for calculating solubility of water in hydrocarbons. See *Thermodynamics: Water K-Values in Hydrocarbon Systems* for details.

Flash Command Summary

Calculation Options

ISOthermal
HEAt change (H units/t units) =
 or
ADIabatic
 and / or
HEAt change (H units/t units) =
ISEntropic
BUBble point
DEW point
DEW WATER
LIQuid **FRA**ction (**MOL**ar/**MAS**s)
VAPor
LIQuid

Outlet Pressure and Temperature Specifications

TEMperature **OUT** (T units) =
PREssure **OUT** (P units) =

Non-equilibrium Specifications

WATER **ENT**rained in **OIL** (units) =
OIL **ENT**rained in **WATER** (units) =

Lost Work Analysis

TEMperature of **EX**change (T units) =

Separator Sizing Commands

VERTical
HORIzontal
K Constant (L units/t units) =
MISt **ELI**minator
NO MISt eliminator
ALLowable stress (P units) =
JOInt efficiency =
DESign pressure (P units) =
CORrosion allowance (L units) =
WEIght **PER**cent allowance =
RATio of **MAJ**or to minor axes for head =
MINimum level **NOZ**zle height (L units) =
 For vertical vessels only
MINimum **SUR**ge time (t units) =
MINimum **DIS**engaging height (L units) =
MINimum **LIQ**uid to inlet height (L units) =
 For horizontal vessels only
LENgth to **DIA**meter ratio =
MINimum **VAP**or height (L units) =
RESidence time (t units) =
BOOt **DIA**meter (L units) =
Thermodynamics Commands
HKEy =
KKEy =
DKEy =

Flash Step by Step

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Flash STEP 1

Equipment name and connectivity (ALL are required).

Equipment module identifier
 Equipment number
 Equipment name
 Inlet stream
 Outlet streams

FLA
 Assigned equipment flowsheet number
 User choice - up to 16 characters
 One only
 Two or three

Outlet stream specifications

- If two outlet streams are coded, vapor is put into the first outlet stream and hydrocarbon liquid plus soluble water in the second.
- If three outlet streams are coded, the first contains vapor, the second contains hydrocarbon liquid and soluble water and the third contains "free water" plus soluble hydrocarbons.

Flash STEP 2

Choose flash type. Calculation Options (select ONE only)

- Isothermal flash (two algorithms are available; the FLash algorithm and the MULTiple FLash algorithm.)
 - Request FLash algorithm (default) **ISO**
 - or
 - Request MULTiple FLash algorithm
- Adiabatic flash (two algorithms are available; the FLash adiabatic algorithm and the MULTiple FLash algorithm.)
 - Request FLash adiabatic algorithm **HEA** (H units/t units) =
 - or **ADI** and/or
 - Request MULTiple FLash algorithm **HEA** (H units/t units) =
 - Isentropic flash **ISE**
 - Bubble point **BUB**
 - Dew point **DEW**
 - Water dew point (IMM = 62 required) **DEW** **WAT**
 - Liquid fraction (default unit is MOLar) **LIQ** **FRA** (**MOL**ar/**MAS**s units) =
 - Vapor phase **VAP**

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Liquid phase

LIQ

Outlet pressure and temperature specifications (select ONE of the following)

Pressure out

PRE OUT (P units) =

Temperature out

TEM OUT (T units) =

NOTE: These specifications may not be used with the FLAsh isothermal and adiabatic algorithms. In all other cases outlet stream specifications are required. If you do not specify outlet temperature and pressure, the inlet conditions will be used as needed. In the event of over specification, temperature will be varied.

Non-equilibrium Separation

- Water entrained in oil
- Oil entrained in water

WAT ENT OIL (units) =

OIL ENT WAT (units) =

where units refers to MOLar fraction, VOLume fraction, or MASs fraction.

NOTE: When three outlet streams are specified there are two options for calculating the solubility of water in hydrocarbons. See *Thermodynamics: Water K-Values in Hydrocarbon Systems* for details.

Flash STEP 3

Lost Work Analysis

Temperature of heat exchange fluid (use only with LOST WORK analysis, default is 250 F for heating, 70.3 F for cooling)

TEM EXC (T units) =

Separator Sizing

One of these is sufficient to obtain sizing results using default values

Vessel orientation

VERT or **HORI**

Sizing is also performed if any of the following commands are used, in which case the vessel is assumed to be VERTICAL unless otherwise specified. Reasonable default values are supplied by the program for unspecified commands.

K constant, velocity (default is 0.35)

K CO (L units/t units) =

Mist eliminator, six inch (default)

MIS ELI

No mist eliminator

NO MIS

Allowable stress (default is 15014.7 PSIA)

ALL (P units) =

Joint efficiency (default is 1.0)

JOI =

Design pressure (default is 10% higher than inlet)

DES (P units) =

Corrosion allowance (default is 0.125 inches)

COR (L units) =

Weight percent allowance (default is 20.0)

WEI PER =

Ratio of major to minor axes for heads (default is 2.0)

RAT MAJ =

Minimum level nozzle height (default is 1.5 feet)

MIN NOZ (L units) =

Length of the shell

LEN SHE (L units) =

For a vertical vessel only, you can specify the following:

Surge time (default is 2 minutes)

SUR (t units) =

Minimum disengaging height (default is 3 feet)

MIN DIS (L units) =

Minimum distance between the inlet nozzle and the high liquid level (default is 2 feet)

MIN LIQ (L units) =

For a horizontal vessel only, you can specify the following:

Ratio of length to diameter (default is 4.0)

LEN DIA =

Minimum vapor height (default is 1.25 feet)

MIN VAP (L units) =

Residence time (default is 5 minutes)

RES (t units) =

Boot diameter (no default)

BOO DIA (L units) =

IF thermo is different from global (GENeral section) options THEN select:

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Flash Separator Sizing

Flash: Sizing Command Details

The sizing calculation is performed if you specify either: **VERTical** or **HORIzontal**

One of these is sufficient to obtain sizing results using default values. Sizing is also performed if any of the following commands are used, in which case the vessel is assumed to be VERTICAL unless otherwise specified. Reasonable default values are supplied by the program for unspecified commands.

K COnstant (L units/t units) =

Enter the K COnstant (velocity). Default is 0.35. See Table 1

MIST ELiminator

Enter this command to specify that the vessel has a mist eliminator. Default option.

NO MIST eliminator

Enter this command to indicate that there is not a mist eliminator in the vessel.

ALLowable stress (P units) =

Enter the allowable stress. Default is 15014.7 PSIA.

JOint efficiency =

Enter the joint efficiency. Default is 1.0.

DESign pressure (P units) =

Enter the design pressure. Default is 10 percent higher than the operating pressure.

CORrosion allowance (L units) =

Enter the corrosion allowance. Default is 0.125 inches.

WEight **PER**cent allowance =

Enter the weight percent allowance. Default is 20.0

RATio of **MAJ**or to minor axes for head =

Enter the ratio of major to minor axes for the heads. Default is 2.0.

MINimum level **NOZ**zle height (L units) =

Enter the minimum level nozzle height from tangent line to high liquid level. Default is 1.5 feet. This command can be used to ensure that your vessel has sufficient liquid level for proper placement of level control nozzles.

LENgth of **SHE**ll (L units) =

Enter the length of shell. There is no default value for this command.

For a vertical vessel only, you can specify the following commands:

minimum **SUR**ge time (t units) =

Enter the minimum surge time. This will be used to determine the high liquid level measured from the tangent line of the vessel. Default is 2 minutes.

MINimum **DIS**engaging height (L units) =

Enter the minimum disengaging height. Default is 3 feet.

NOTE: The lower limit for this specification is the diameter of the vessel.

MINimum **LIQ**uid to inlet height (L units) =

Enter the minimum distance between the inlet nozzle and the high liquid level. Default is 2 feet.

NOTE: The actual distance between the inlet nozzle and the high liquid level is at least one half the vessel diameter. It will be increased, if necessary, to satisfy both the minimum liquid to inlet height and the total vessel length.

For a horizontal vessel only, you can specify the following commands:

DIAmeter (L units) =

Enter the diameter of the vessel. Default is none.

If diameter is specified, program will calculate the residence time.

LENgth to **DIA**meter ratio =

Enter the ratio of length to diameter. Default is 4.0. This ratio is used to calculate the length of the vessel.

MINimum **VAP**or height (L units) =

Enter the minimum vapor height. Default is 1.25 feet.

RESidence time (t units) =

Enter the residence time. Default is 5 minutes.

If residence time is specified, program will calculate the diameter of the vessel.

NOTE: The default unit for time is hours. The residence time will be used to determine the normal minimum liquid level. This should include any additional settling time needed for separation of two liquid phases.

BOOt **DIA**meter (L units) =

Enter the boot diameter if you want to separate two liquid phases in the vessel. The second liquid phase will be contained in the boot. The program will calculate the size of the horizontal vessel required for the vapor and first liquid phase and the length of the boot for the second liquid phase. There is no default value.

Flash: Methods and Assumptions

Pipe will be used to fabricate the shell for diameters up to 36 inches. Nominal diameters used for pipe in inches are: 8, 10, 12, 14, 16, 18, 20, 24, 26, 28, 30, 32, 34, 36.

Plate steel will be used for diameters over 36 inches. Selected diameters will be multiples of 6 inches for plate steel. Shell lengths selected will be multiples of 2 feet unless length is specified. Boot length will be a multiple of 6 inches. A 6-inch-thick mist eliminator, if used, will permit smaller diameters since the usual 15 percent safety factor on terminal vapor velocity is not needed. With a mist eliminator the vapor velocity can be as high as the terminal vapor velocity calculated from the Souders

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and Brown equation. The mist eliminator, if used, is assumed to be located at the top tangent line of a vertical vessel. No distinction is made between tangent line and seam. Shell heads are semi-ellipsoidal 2:1 unless otherwise specified.

Method of Calculation-Diameter

The diameter needed for separation of vapor and liquid is estimated using the Souders and Brown equation. This uses fluid densities which are automatically obtained from the outlet streams on the flowsheet. In the case of a compressor suction or inlet gas separator, where there is no liquid at operating conditions, the liquid density used is obtained from a dew point calculation. If there are two liquid phases the program uses average liquid properties unless a boot is specified for the second liquid phase.

For vertical separators the diameter is selected to meet both separation and surge time criteria. For horizontal separators two diameters are reported. The first is the diameter needed to perform the separation with the vessel half full of liquid. The second diameter is the one actually selected which also satisfies the liquid residence time specification. Liquid level is determined in conjunction with this diameter to meet the following design recommendations (*Flash References*: Reference 1):

- Vapor space should be in the range 15 - 50 percent of cross-sectional area.
- Vapor height should be at least the minimum specified or default of 15 inches.

Layout considerations often require the length of a horizontal vessel to be fixed by the user. In this case the diameter is increased if necessary to meet the other specifications. Minimum vessel diameter is 8 inches.

Pipe is selected for vessel fabrication where diameter (up to 36 inches) and wall thickness permit. Otherwise plate steel is chosen in a suitable thickness which is a multiple of 1/16 inches. Wall thickness for pipe is selected from one of STD, XS, XXS (if available) pipe wall codes or the maximum manufactured thickness in each pipe size.

NOTE: The K COnstant largely determines the vessel diameter, so the value you enter should be based on your engineering judgment and experience. The default value of 0.35 is suitable for vertical separators with a 6-inch mist pad for hydrocarbons in low pressure service. For horizontal vessels, you generally multiply the vertical K COnstant by 1.25. For vessels containing glycol or amine solutions, you generally multiply the K constant by 0.82. *See Table 1. Typical K Constants* below.

The following suggestions are intended only as general guidelines for vertical vessels in hydrocarbon service:

Table 1. Typical K COnstants

Service	K COnstant for vertical	K COnstant for horizontal
Hydrocarbons at: 0 PSIG	0.36	0.45
100 PSIG	0.35	0.44
300 PSIG	0.33	0.41
600 PSIG	0.30	0.38
900 PSIG	0.27	0.34
1500 PSIG	0.21	0.26
Wet steam, 0-1500 PSIG	0.25	0.31
Most vapor under vacuum	0.20	0.25
Salt and caustic evaporators	0.15	0.19

Method of Calculation-Length

For vertical vessels, the length is calculated from the sum of the high liquid level, the liquid-to-inlet height, the disengaging space and the mist eliminator thickness. The high liquid level is calculated from the minimum surge time and adjusted if necessary to meet the minimum nozzle height requirement. The actual disengaging space is the minimum disengaging height or the vessel diameter, whichever is larger. The actual liquid-to-inlet nozzle height may be larger than the minimum liquid to inlet height since it is at least one half of the vessel diameter. It is also adjusted if necessary to meet the total vessel length, which is in multiples of 2 feet if not specified.

For horizontal vessels the length is calculated from the length to diameter ratio. If length is specified, diameter is adjusted to meet other specifications. If the vessel has a boot, the boot length is calculated from the second liquid volume and rounded to multiples of 6 inches.

Method of Calculation - Boot

The boot calculation is only performed on horizontal vessels. The boot is used to separate the second liquid phase from the first liquid phase, so if there is only one liquid phase, the boot is ignored.

The main vessel shell is sized using the vapor and first liquid phase. The length of boot needed for the second heavier liquid phase is then calculated using the specified boot diameter. Weights reported include both the horizontal shell and the boot.

Method of Calculation - Nozzles

Nozzles are sized to meet minimum and maximum velocities calculated by the program according to the recommendations of the *Gulf Publishing Pocket Engineer's Handbook* (*Flash References*: Reference 2).

A sonic velocity check is also made on the inlet and vapor nozzles. Sonic velocity in the gas phase is estimated using the generalized sonic velocity correlation of Sherwood (*Flash References*: Reference 3) for compressed gases.

Method of Calculation - Thickness and Weight

Minimum thickness is calculated from internal design pressure for both shell and ellipsoidal heads (Reference 6). An allowance for corrosion is included in the minimum thickness reported. The corrosion allowance may be specified by the user. The default corrosion allowance of 0.125 inches represents about 24 years of operating life at a typical steel vessel corrosion rate of .0052 inches per year (**Flash References:** Reference 4).

Pipe is selected for vessel fabrication for diameters up to 36 inches, provided that pipe is available in thickness larger than the minimum required thickness. Plate steel is selected for larger diameters.

Pipe wall thickness is chosen from pipe wall codes **STD**, **XS**, **XXS** (if available) and the thickest manufactured wall in each pipe size. If thicker wall is needed, then plate steel is used. Thickness selected for plate steel is in multiples of 1/16 inch. The vessel weight includes the shell and both ellipsoidal heads. If there is a boot, the secondary shell is also included. Both empty and full weights are reported. The full weight is calculated assuming that the vessel is full of liquid at operating conditions. Weights are estimated using a steel density of 489.02 lb/ft³ and an extra percentage allowance for supports and fittings. The user can optionally specify the percentage allowance; otherwise, 20 percent is used.

Flash Examples

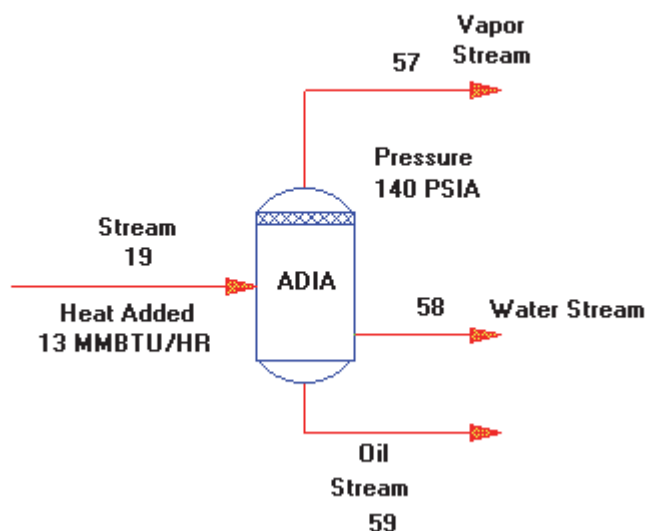
There are several sample flowsheets in "Chapter 23: Flash Samples - c:\designii\samples\equipment\flash" of the DESIGN II for Windows Tutorial and Samples Guide.

Flash: Multiple Flash Algorithm for Adiabatic Flash

```
*MULTIPLE FLASH ALGORITHM
FLash 7 = ADIB, 19, -57, -58, -59
      ADIabatic,
      HEAt added = 1.3E7,
      PREssure OUT = 140
GENeral,
      COMponents = 3, 4, 5,
      FLOW 19 = 400, 100, 200,
END
```

Partial output for Example 5 is shown on the following page.

```
+ EQUIPMENT SUMMARY -
  INDIVIDUAL DETAILS +
****FLASH SEPARATORS ****
EQUIPMENT NO.          7
EXTERNAL NAME          ADIB
TYPE                   ADIABATIC
DUTY                   BTU/HR      1.30000E 07
SPECIFICATION
P OUT   PSIA          140.00
```



Flash References

1. Gerunda, A., How to Size Liquid-Vapor Separators, *Chemical Engineering*, Volume 88, pp. 81-84, May 4, 1981.
2. *The Process Engineer's Pocket Handbook*, Chapter 1, Gulf Publishing Co., Houston, Texas, 1976.
3. Sherwood, T.K., Velocity of Sound in Compressed Gases, *Journal of Chemical & Engineering Data*, Volume 7, No. 1, pp. 47-50, January, 1962.
4. Megyesy, Eugene F., *Pressure Vessel Handbook*, 5th Edition, Pressure Vessel Handbook Publishing, Inc., Tulsa, Okla., 1981.
5. *A.S.M.E. Boiler and Pressure Vessel Code*, Section VIII, Division 1, American Society of Mechanical Engineers, New York.
6. Perry, R.H., and Chilton, C.H., *Chemical Engineer's Handbook*, 5th edition, Chapters 5 & 18, McGraw-Hill Book Company, 1973.

Chapter 19: Flow Meter

This equipment module is applicable to the orifice type flow meter and allows the engineer to calculate the size of the orifice, flow rate of the stream, or the pressure drop across the orifice. Additionally, this model can provide tables and parametric plots of flow rate versus pressure drop. The flow condition can be single or two phase in the subsonic region and vapor phase only in the sonic flow region.

The model allows square-edge, quadrant, and conical type orifice plates. The International Standard Organization method and the American Gas Association methods are available to correlate discharge coefficient and expansion factor for square-edged orifice. This model can accommodate flange, corner, radius, or pipe orifice taps. See *Flow Meter: Range of Application* for orifice and tap types.

NOTE: The input order in this module is not totally free-format. Commands should be entered in the order that they are organized in the DESIGN II Keyword Commands section.

Flow Meter Command Details

Flow Meter: Specify Configuration

FMTR

Specifies the Flow Meter unit operation.
One inlet stream and one outlet are allowed.

ORifice

Enter this command to specify the flow meter type. Default has already been set as orifice. Future releases will allow other types of flow meters.

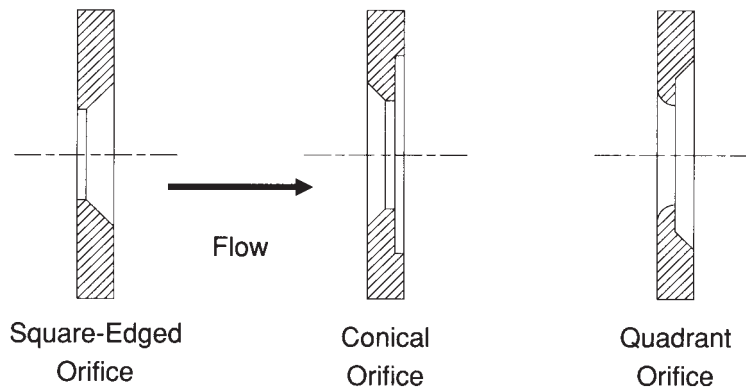
TYPE of orifice =

Enter your choice of orifice type. Options are:

SQUared-edged (default)

QUAdrant

CONical



Type of TAP =

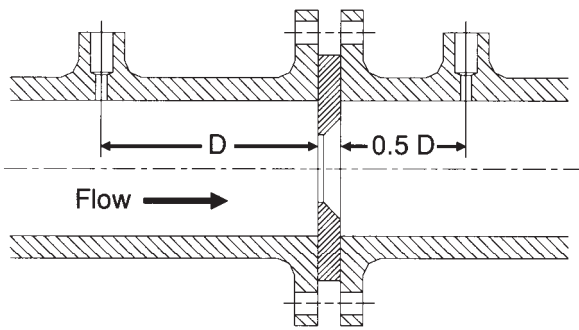
Enter your choice of tap type. Options are:

FLAnge (default)

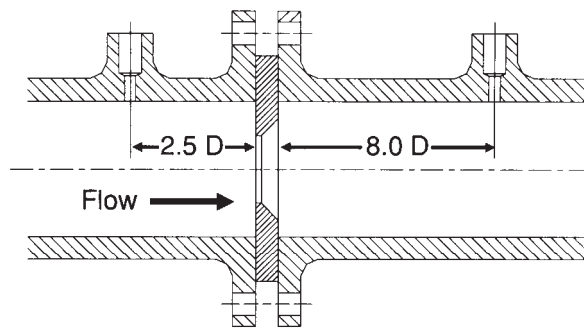
CORner

RADius

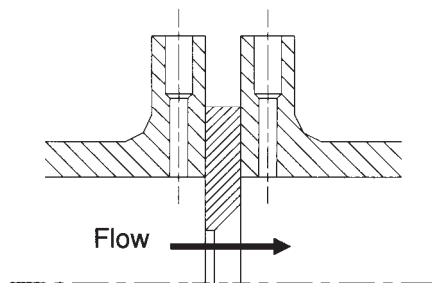
PIPe



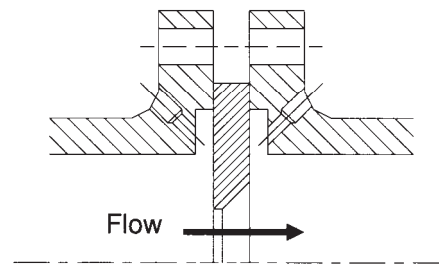
Radius Tap



Pipe Tap



Flange Tap



Corner Tap

Flow Meter: Specify the Pipe Configuration

The pipe configuration can be defined by either specifying the nominal diameter and pipe wall thickness code or by specifying the inside diameter alone.

PIPE WALL thickness code =

Enter the desired pipe wall thickness code. Options are:

STD (standard wall) (default)

XS (extra strong wall)

XXS (double extra strong wall)

NOMinal **DIAM**eter (L units) =

Enter the nominal diameter for the pipe. See *Table 2 in Size Lines*. They are consistent with Crane Technical Paper No. 410.

or

INSide **DIAM**eter (L units) =

Enter the inside diameter of the pipe.

Flow Meter: Specify the Discharge Coefficient and the Expansion Factor Method

METhod of computation =

Enter the choice of computation method.

Options are:

ISO available for flange, corner, radius and pipe taps. (default)

AGA available for flange and pipe taps only if a square edge orifice is specified.

API available for flange and square-edged orifice meters only.

Flow Meter: Specify Desired Computation Option

CALculate **FLOW** rate

Enter this command to compute the flow rate. The **DIAM**eter of the flow meter (or **RAT**io) and the **DEL**ta pressure must be specified.

CALculate **SIZE**

Enter this command to compute the diameter of the flow meter. The **FLOW** **RAT**e and the **DEL**ta pressure must be specified.

CALculate delta **PRE**ssure

Enter this command to compute the delta pressure of the flow meter. The **DIAM**eter of the flow meter (or **RAT**io) and the **FLOW** **RAT**e must be specified.

Flow Meter: Specify Process Information

DIAMeter of flow meter (L units) =

Enter this command to specify the diameter of the flow meter. Not required if the **CALculate SIZE** keyword is specified.

or

RATio of the flow meter and pipe diameter =

An alternative to specifying the diameter of the flow meter is to specify the ratio of flow meter diameter to the inside diameter of the pipe.

FLOW RATE (Q/Time units) =

Enter this command to specify the flow rate. This is a specification and is not necessarily the same as the feed stream flowrate. Not required if **CALculate FLOWrate** is specified.

DELta pressure (P units or INH2O) =

Enter this command to specify the differential pressure. Not required if **CALculate delta PREssure** is specified.

Flow Meter: Specify Output Information

PLOt RATio = r1,..., rn

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified flow meter to pipe diameter ratios (r1,...rn). **RANge** of **DELta** pressure must also be specified.

PLOt TEMperature (T units) = t1, ..., tn

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified upstream temperature (t1,...tn). **RANge** of **DELta** pressure must also be specified with this command.

PLOt PRESSure (P units) = p1, ..., pn

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified upstream pressure (p1,...pn). **RANge** of **DELta** pressure must also be specified with this command.

RANge of **DELta** pressure (P units or INH2O) = DPmin, DPmax

Enter this command to specify the desired range of differential pressure.

TABLE OFF

Enter this command to turn off the tabular output. (output plot only)

PLOt OFF

Enter this command to turn off the parametric plot. (table only)

PRInt RECycle

Enter this command to provide flow meter output for each iteration of a recycle loop. Default is no flowmeter output during recycle iterations.

Flow Meter Calculation Method

Given two flow meter parameters (size, flow or pressure drop) the program calculates the third parameter based on the fluid characteristics listed in the links below. The program provides flow meter results on two columns. One for the **SPECIFIED CALCULATION** option chosen by the user and the other as **ACTUAL FLOWRATE** column. The pressure drop under the actual flowrate column is the pressure drop due to the orifice as measured downstream (beyond the vena contracta point) whereas the pressure drop under the specified calculation column is the pressure drop measured by the flow meter at the specified case. The total pressure drop due to the flow meter should be less than the measured pressure drop.

Note: Actual pressure drop is the estimated drop between upstream tap and downstream pressure.

Flow Meter: Single Phase Flow in the Subsonic Region

The orifice meter flow equation used in this case is:

$$Q = \frac{C}{[1-\beta^4]^{1/2}} Y \frac{\pi}{4} d^2 [2g_c \rho_f \Delta P]^{1/2}$$

where

Q	mass flow rate
C	discharge coefficient
Y	expansion factor
β	ratio of orifice diameter to measured pipe diameter
d	orifice diameter
g_c	dimensional conversion constant
ΔP	differential pressure across orifice
ρ_f	density of fluid

The reference for computing discharge coefficient and expansion factor is given in *Flow Meter: Range of Application*

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Flow Meter: Two Phase Flow in the Subsonic Region

The orifice meter equation (Reference 5) used in this regime is:

$$Q = \frac{K_g Y_g \frac{\pi}{4} d^2 \sqrt{2 g_c \rho_g \Delta P}}{(1-y) + 1.26 y \frac{K_g Y_g}{K_1} \sqrt{\frac{\rho_g}{\rho_1}}}$$

where

Q mass flow rate

$$K_1 = \frac{C_1}{(1-\beta^4)^{1/2}}$$

$$K_g = \frac{C_g}{(1-\beta^4)^{1/2}}$$

y liquid fraction
 C_g, C_1 discharge coefficient gas, liquid
 Y expansion factor
 d orifice diameter
 g_c dimensional conversion constant
 ΔP differential pressure across orifice
 ρ_g, ρ_1 density of gas, liquid

Flow Meter: Vapor Phase Flow in the Sonic Region

The orifice meter flow equation (Reference 1) used in this regime is:

$$Q = 0.6098863 * C d^2 Y_{cr} \sqrt{\frac{G}{T_{f1}} F_{tp} P_{f1}}$$

where

Q mass flow rate
 C discharge coefficient
 d orifice diameter
 Y_{cr} expansion factor at critical flow
 G gas specific gravity (molecular weight of gas / molecular weight of air)
 T_{f1} upstream temperature
 F_{tp} factor correcting static pressure to total pressure
 P_{f1} upstream pressure

Flow Meter: Range of Application

The following table lists the range of application for the available orifice plate and tap types and the available methods for calculating the discharge coefficient and expansion factor.

Method	Tap Type	Pipe Diameter	Beta-Ratio or Diameter of Orifice	Reynold's Number (Rd* or RD*)
ISO	flange, corner, radius	2 inch < D < 36 inch	$0.2 < \beta < 0.75$	2,000 - 10,000,000 (RD)
(square-edged orifice)	pipe	2 inch < D < 36 inch	$0.2 < \beta < 0.70$	10,000 - 10,000,000 (RD)
AGA	flange	D > 1.6 inch	$0.1 < \beta < 0.75$	---
(square-edged orifice)	pipe	D > 2 inch	$0.2 < \beta < 0.67$	---
Quadrant	flange, corner, radius	D > 2 inch	0.225 0.4 0.5 0.6 0.63	5,000 - 60,000 (Rd) 5,000 - 150,000 (Rd) 4,000 - 200,000 (Rd) 3,000 - 150,000 (Rd) 3,000 - 105,000 (Rd)
Conical	n/a	n/a	D > 0.25 in. $\beta < 0.316$	250 - 200000 (Rd)

- **RD** is the Reynold's No. based on the pipe diameter D. **Rd** is the Reynold's No. based on the orifice diameter d.

Flow Meter Command Summary

Configuration Commands

FMTR

ORIfice

TYPE of orifice =

SQUared-edged (default)

QUAdrant

CONical

Type of **TAP** =

FLAnge (default)

CORner

RADius

PIPe

Calculation Commands

CALculate **FLO**w rate

CALculate **SI**ze

CALculate delta **PRE**ssure

Output Commands

PLOt RATio = r1,..., rn

PLOt TEMperature (T units) = t1, ..., tn

PLOt PREssure (P units) = p1, ..., pn

RANge of **DEL**ta pressure (P units or INH2O) = DPmin, DPmax

TABLE OFF

PLOt OFF

PRInt RECycle

Process Commands

DIAmeter of flow meter (L units) =

or

RATio of the flow meter and pipe diameter =

FLOw RATe (Q/Time units) =

DELta pressure (P units or INH2O) =

Method of Calculation Commands

METHod of computation =

Options are:

ISO available for flange, corner, radius and pipe taps. (default)

AGA available for flange and pipe taps only if a square edge orifice is specified.

API available for flange and square-edged orifice meters only.

Pipe Configuration Commands

PIPe WALI thickness code =

Options are:

STD (standard wall) (default)

XS (extra strong wall)

XXS (double extra strong wall)

NOMinal **DIA**meter (L units) =

or

INSide **DIA**meter (L units) =

Flow Meter Step by Step

Flow Meter STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet. Equipment name and connectivity (ALL are required).

Equipment module identifier	FMTR
Equipment number	Assigned equipment flowsheet number
Equipment name	User choice - up to 16 characters
Inlet stream	One only
Outlet streams	One only

Flow Meter STEP 2

Specify the Flow Meter Configuration Commands.

Flow Meter Type	OR Ifice =
Type of orifice	TYPE = SQU ared-edged (default) QUA drant CON ical
Type of Tap	TAP = FLA nge (default) COR ner RAD ius PIPe

Flow Meter STEP 3

Choose the Pipe Configuration listed below.

Pipe Wall Thickness Code	PIPe WALl thickness = STD (standard wall - default) XS (extra strong wall) XXS (double extra strong wall)
Enter the nominal diameter for the pipe. OR	NOM inal DIA meter (L units) =
Enter the inside diameter of the pipe.	INS ide DIA meter (L units) =

Flow Meter STEP 4

Enter the Discharge Coefficient and Expansion Factor Method.

Enter the choice of computation method.	METH od of computation =
Options are:	
ISO available for flange, corner, radius and pipe taps. (default)	ISO
AGA available for flange and pipe taps only if a square edge orifice is specified.	AGA
API available for flange and square-edged orifice meters only.	API

Flow Meter STEP 5

Specify the desired Computation Options to estimate a variable among the three below. Enter ONE of the following calculation commands based on the other two specified variables.

Enter this command to compute the flow rate. The DIAMeter of the flow meter (or RATio) and the DELta pressure must be specified. **CAL**culate **FLOW** rate

Enter this command to compute the diameter of the flow meter. The FLOW RATE and the DELta pressure must be specified. **CAL**culate **SIZE**

Enter this command to compute the delta pressure of the flow meter. The DIAMeter of the flow meter (or RATio) and the FLOW RATE must be specified. **CAL**culate delta **PRE**ssure

Flow Meter STEP 6

Specify the Process Information

Enter this command to specify the diameter of the flow meter. Not required if the CALculate SIZE keyword is specified. **DIAM**eter of flow meter (L units) =

OR

An alternative to specifying the diameter of the flow meter is to specify the ratio of flow meter diameter to the inside diameter of the pipe. **RAT**io of the flow meter and pipe diameter =

Enter this command to specify the flow rate. This is a specification and is not necessarily the same as the feed stream flowrate. Not required if CALculate FLOWrate is specified. **FLOW RATE** (Q/Time units) =

Enter this command to specify the differential pressure. Not required if CALculate delta PREssure is specified. **DEL**ta pressure (P units or INH₂O) =

Flow Meter STEP 7

Specify the Output Information

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified flow meter to pipe diameter ratios (r1,...,rn). RANGE of DELta pressure must also be specified. **PLOt RAT**io = r1,..., rn

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified upstream temperature (t1,...,tn). RANGE of DELta pressure must also be specified with this command. **PLOt TEM**perature (T units) = t1, ..., tn

Enter this command to generate a plot and table for flow rate versus delta pressure for the specified upstream pressure (p1,...,pn). RANGE of DELta pressure must also be specified with this command. **PLOt PRE**ssure (P units) = p1, ..., pn

Enter this command to specify the desired range of differential pressure. **RAN**ge of **DEL**ta pressure (P units or INH₂O) = DPmin, Dpmax

Enter this command to turn off the tabular output. **TABLE OFF**

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(output plot only)

Enter this command to turn off the parametric plot. **PLOt OFF**
(table only)

Enter this command to provide flow meter output for each iteration of a recycle loop. Default is no flow meter output during recycle iterations. **PRInt RECycle**

IF thermo is different from global (GENeral section) options THEN select:

K-value option **KKE =**

Enthalpy option **HKE =**

Density option **DKE =**

Flow Meter Examples

There are several sample flowsheets in "Chapter 24: Flow Meter Samples - c:\designii\samples\equipmnt\flowmetr" of the DESIGN II for Windows Tutorial and Samples Guide.

Flow Meter References

1. Miller, R. W., *Flow Measurement Engineering Handbook*, McGraw-Hill Book Company, 1983.
2. *API, Manual of Petroleum Measurement Standards*, Chap. 14 - Natural Gas Fluids Measurement, Section 3 - Orifice Metering of Natural Gas and Other Related Hydrocarbon Fluids, American Petroleum Institute, Washington, D.C., 1985.
3. Perry, R. H. and Green, D., *Perry's Chemical Engineering Handbook*, McGraw Hill Book Company, 1984.
4. British Standard 1042, *Methods for the Measurement of Fluid Flow in Pipes, Part 1. Orifice Plates, Nozzles and Venturi Tubes*, UDC 532.54.08, British Standards Institution, London, 1964.
5. Murdock, J. W., "Two-Phase Flow Measurement with Orifices," *Journal of Basic Engineering*, Dec. 196, p.419, 196.
6. *API, Manual of Petroleum Measurement Standards*, Chap. 14, Section 3, part 1.7.2., American Petroleum Institute, Washington, D.C., August 1990.

Chapter 20: Heat Exchanger

The HEAt EXChanger module can be used to specify heating or cooling of a stream or to calculate counter current heat exchange between two streams. The module calculates the heat and material balance from known input stream information and the specification to be met.

Heat Exchanger Features

TYPES OF EXCHANGERS

The following types of exchangers are described:

- Single Stream Temperature Change
- Counter-Current Heat Exchange
- Air Cooled Heat Exchange
- Water Cooled Heat Exchange
- Refrigerant Heat Exchange

In the discussion of each of these types of exchanger, guidelines are presented as to when and how they should be used. To select the appropriate type, first determine what input information you have, and what information you want to have calculated. For example, do you need all the information about both sides of the exchanger, or are you just trying to set the temperature of your process stream?

Do you need to know everything about the heat exchanger now, or could you wait until you finish your design of the process, then go back and get all the information on the exchanger.

Stream Order

The HEAt EXChanger module always applies your specification to the first stream in and out. The pressure drop command contains information for both the first and second outlet streams. The order in which the streams are coded determines the stream to which your specifications will be applied. For instance:

```
HEAt EXChange 1 = E101, 3, 1, -4, -2, TEMperature OUT = 70
```

In the above example, to specify the temperature of stream 4 to be .70 F, you must code stream 4 as the first output stream.

Assumed Input

The HEAt EXChanger module assumes that all the properties of the inlet streams are known. Properties such as temperature, pressure, enthalpy, and component flowrates must be known in order to calculate the heat exchange. If one of the inlet streams is not known at the time the module is calculated, the calculation is not performed, and the known properties of the inlet stream are transferred to its outlet.

Setting Stream Temperature and Pressure

The HEAt EXChanger can be used to set the temperature and pressure of a process stream. The module is coded with one stream in and one stream out. A pressure drop (which can be negative or positive) can be specified along with the outlet temperature. For example, if the temperature of a stream is 200 F and the pressure is 200 PSIA and you wish to set the pressure to 600 PSIA, the coding would look like this:

```
HEAt EXchanger 1 = E101, 1 -2, TEMperature OUT = 200, DELta = -400
```

Duties

To specify heat addition to a stream, you use the DUTy command with a positive value for the heat addition. A negative value indicates heat removed. The output for the exchanger will report a positive Q for heat added to the first inlet stream or a negative Q for heat removed from the first inlet stream.

Dew or Bubble Point Feeds to the Exchanger

If a feed to a HEAt EXChanger module is to be at its dew point or bubble point, special care should be taken to insure that this condition is achieved by the program and is not just an estimate on your part. For example, if the feed is a pure component or narrow boiling mixture at bubble point, guessing at the temperature and pressure can result in the wrong phase, because the dew point temperature will not be much different than the bubble point. If your guess is off by even a degree, the feed could be half vapor. To make sure your bubble or dew point feeds are at the right temperature and have the proper phase, put them through a HEAt EXChanger module and specify the bubble or dew point to be calculated. Remember, this needs to be done only for feed streams and not intermediate streams that will be calculated by the program.

Heat Exchanger Command Details

Heat Exchanger: Single Stream Temperature Change

In many process simulations only one side of the exchanger is of interest. For example, you may be interested only in process

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stream temperature adjustment, not the amount of the utility required for the heat exchange. For most exchangers using a heating or cooling material to adjust the temperature of a process stream, you can code the exchanger with only one stream in and one stream out and reduce the complexity of the simulation.

Output

The duty and/or temperature out of the exchanger are calculated along with all the properties of the outlet stream.

Heat Exchanger: Single-Stream Exchanger Commands

Specifications Available (enter only one of the following)

TEMperature **OUT** (T units) =

Enter desired temperature of the outlet stream.

DUTy (H units/t units) =

Enter the desired enthalpy change of the input stream. Positive value indicates heating; negative indicates cooling.

TEMperature **OUT** is **BUB**ble point

Sets temperature of the outlet stream to the bubble point.

TEMperature **OUT** is **DEW** point

Sets temperature of the outlet stream to the dew point.

TEMperature **AP**proach (T units) =

Absolute temperature difference between the shellside outlet stream and the tubeside inlet stream (must be greater than 2° F).

DELta **TEM**perature (T units) =

Enter the desired change in temperature from inlet to outlet. Positive value indicates heating; negative indicates cooling.

Heat Exchanger: Single Stream Exchanger Optional Commands

If a stream is being cooled in a single stream exchanger, the program will automatically try to use water for the cooling. It will use water if the process stream is cooled to a temperature which is at least 10 F (5.56 K) warmer than the inlet water temperature, which has a default value of 90F(305.4 K).

The following optional commands can be used to set the cooling water temperatures:

TEMperature of **WAT**er **IN** (T units) =

Enter the temperature of the inlet cooling water. Default is 90 F (305.4 K). Water needed for cooling is automatically calculated if the temperature of the process stream is greater than water temperature in.

TEMperature of **WAT**er **OUT** (T units) =

Enter the temperature of the cooling water out of the exchanger. Default is TEM WAT IN plus 15 F (8.33 K).

Heat Exchanger: Counter-Current Commands

This exchanger simulates two process streams exchanging heat with each other, usually a heat recycle situation with one of the streams coming from downstream in the process.

For counter-current exchangers, remember to keep your input and output streams in the correct order, make sure your streams are coded so the specification is applied to the correct stream, and review your problem to see if the heat recycle can be removed.

If a **SIM**ple exchanger is specified, the surface area and overall heat transfer coefficient of the exchanger should also be specified. If not, the area per shell will default to 100 FT² and the overall heat transfer coefficient will default to 50 BTU/HR/FT²/ F

Output

All outlet stream properties are calculated. The duty, area per shell, and corrected log mean temperature difference are reported. This is an iterative process which would require more execution time than a **TEM**perature **OUT** or **DUT**y specification.

Specifications Available (enter only one of the following)

SIMple exchanger

AREa and given U are used to calculate the temperatures out. Specify the AREa and U commands with this option

AREa (L units) =

Enter the area per shell for the **SIM**ple exchanger specification. Default is 100 FT² (9.29 M²).

and

SHElls in **PAR**allel =

Enter the number of parallel shells. This command is **ONLY** valid for parallel shells when used in **RAT**ed heat exchangers. When no **RAT**ing is performed, this command is not used. Default is 1.

SHELLs in SERies =

Enter the number of shells in series. This command is valid for series shells when used in non-RATed heat exchangers. When RATING is performed, the only configuration allowed is two E shells in which case it is 2 (see Figure 2 in [Heat Exchanger: Tube Commands](#)). Default is 1.

SHELL PASSes =

Enter the number of shell passes per shell. Default is 1. (First inlet stream coded is shellside.)

U (U units) =

Enter the overall heat transfer coefficient. Default is 50 BTU/HR/FT²/ F (0.2839 KJ/SEC/M²/ K).

TEMPerature OUT Shell Side (T units) =

Enter desired temperature of the stream coded as the first outlet stream. This is for shell side outlet stream.

TEMPerature OUT TUBE Side (T units) =

Enter desired temperature of the tube side outlet stream.

DUTy (H units/t units) =

Enter the desired enthalpy change (- for cooling, + for heating) of the stream coded as the first input stream.

Shell Side TEMPerature OUT is BUBble point

Sets temperature of stream coded as the first outlet stream to the bubble point. This is for shell side outlet stream.

Shell Side TEMPerature OUT is DEW point

Sets temperature of stream coded as the first outlet to the dew point. This is for shell side outlet stream.

TEMPerature APPROach (T units) =

Absolute temperature difference between stream coded as the first outlet stream and stream coded as the second input stream (must be greater than 2 F). Note that the order of streams is with respect to the shell and tube side streams on flowsheet.

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 (please see [Calculation Options: Heat Exchanger Temperature Crossover](#)).

Shell Side DELta TEMPerature (T units) =

Enter the desired change in temperature from inlet to outlet. +ve value indicates heating; -ve value indicates cooling. This specification is for the shell side outlet stream.

Heat Exchanger: Counter-Current Optional Commands

NOTE: The rating commands are listed in this section under Heat Exchanger Optional Command Details. If you enter a value for AREa which is inconsistent with the area calculated from exchanger geometry your specified AREa will be used.

Heat Exchanger: Water Cooled Exchangers

Water-cooled exchangers are handled as single-stream exchangers. The water temperatures in and out are specified by commands in the HEAt EXChanger section rather than TP commands in the GENERAL section.

The amount of water is calculated as part of the HEAt EXChanger output rather than specified on a FLOW command or reported in the final stream summaries. Therefore, the water stream in and out of the water cooled exchanger does not need to be numbered nor included as part of the flowsheet. Also, the identification number for water does not have to be coded on the COMPONENTS command in the GENERAL section.

Heat Exchanger: WATER COOled Exchanger Commands

The WATER COOled exchanger allows you to specify the AREa and U of the exchanger. This option would normally be used to simulate an existing water cooled exchanger where the area is known and the required water must be calculated. This is an iterative calculation and could take up to six times longer to solve than other exchanger types.

Output

The amount of water required is calculated along with the duty, corrected LMTD and outlet stream properties for the process stream. (enter all of the following)

WATER COOled exchanger

Uses the specified AREa and U to calculate water required and outlet temperature of the process stream.

U (U units) =

Enter the overall heat transfer coefficient. Default is 50 BTU/HR/FT²/ F (0.2839 KJ/SEC/M²/ K).

AREa (L2 units) =

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Enter the area per shell for the WATER COOled exchanger option. Default is 100 FT² (9.29 M²).

The following Optional Commands can be used to set the cooling water temperatures:

TEMperature of **WATER IN** (T units) =

Enter the temperature of the inlet cooling water. Default is 90 F (305.4 K).

TEMperature of **WATER OUT** (T units) =

Enter the temperature of the cooling water out of the exchanger. Default is TEM WAT IN plus 15 F (8.33 K).

Heat Exchanger: Water Cooled Condenser Commands

WATER COOled CONDenser

Calculates water required to totally condense the process stream. The WATER COOled CONDenser is used in the specific situation where water is used to condense a process stream to the bubble point. This option would normally be used to simulate total condensers associated with columns or where a product must be liquefied for storage.

Output

The amount of water required to condense the process stream is calculated along with the duty, area, corrected LMTD, and outlet stream properties for the process stream.

Specifications Available

None of the specifications are available since the delta temperature for streams is fixed. The following optional commands can be used to set the cooling water temperatures:

TEMperature of **WATER IN** (T units) =

Enter the temperature of the inlet cooling water. Default is 90 F (305.4 K).

TEMperature of **WATER OUT** (T units) =

Enter the temperature of the cooling water out of the exchanger. Default is TEM WAT IN plus 15 F (8.33 K).

NOTE: The rating commands and guidelines begin in this section under Heat Exchanger Optional Commands. If you enter a value for AREa which does not agree with the area calculated from exchanger geometry, your specified AREa will be used.

Heat Exchanger: Refrigerant Exchangers

Refrigerant exchangers are handled like counter current heat exchangers with the refrigerant entering at the bubble point and leaving at the dew point. Only a single component refrigerant can be handled with the described options. Mixed refrigerant exchangers can be handled by coding the refrigerant stream composition as a feed stream in the GENeral section. The CONTroller module could then adjust the flow via the STream manipulator module until a desired HEAt EXChanger or stream property is obtained (such as the process stream temperature out of the exchanger).

Single component refrigerant exchangers require you to code stream numbers for the refrigerant stream in and out, so the flowrate and properties of the refrigerant can be calculated and reported as part of the final stream summary. Refrigerant stream can be located on the tube or the shell side of a two-stream exchanger. Also the component identification number of the refrigerant must be included on the COMponent command in the GENeral section of the input.

Output

The temperature or pressure of the refrigerant is calculated along with the flowrate required and all properties. The properties of the process stream out are calculated. The duty, area, and corrected LMTD are calculated and reported in the equipment summary.

Heat Exchanger: Refrigerant Exchanger Commands

REFrigerant = **TUBE**

Enter the exchanger feed location for the refrigerant to be on tube side.

REFrigerant = **SHELL**

Enter the exchanger feed location for the refrigerant to be on shell side.

REFrigerant = **COOLED**

Enter if refrigerant is being cooled. Refrigerant is heated, by default.

(enter **ONLY ONE** specification for the refrigerant)

PREssure of **REF**rigerant (P units) **i** =

Enter the pressure at which the refrigerant temperature is to be calculated. **i** is the component identification number for the refrigerant and must appear on the COMponent command in the GENeral section.

TEMperature of **REF**rigerant (T units) **i** =

Enter the temperature at which the refrigerant pressure is to be calculated.. The component identification number for the refrigerant **i** must appear on the COMponent command in the GENeral section.

NOTE: If the pressure is provided, the temperature is calculated. On the other hand, if the temperature is given, the pressure is calculated. Initial guesses for the temperature or pressure of the refrigerant should be given in a TP command in the GENeral section.

REFrigerant SUBcooled (T units) **i** = delta temperature

Enter the amount of subcooling. **i** is the component identification number for the refrigerant and must appear on the COMponent command in the GENeral section.

REFrigerant SUPERheated (T units) **i** = delta temperature

Enter the amount of superheat. **i** is the component identification number for the refrigerant and must appear on the COMponent command in the GENeral section.

(enter **ONLY ONE** specification for the process stream)

DELta TEMperature (T units) =

Enter the desired change in temperature from inlet to outlet. Only negative values are allowed for the refrigerant exchanger. This specification is for the process stream.

TEMperature OUT (T units) =

Enter desired temperature of the process stream.

TEMperature APProach (T units) =

Enter the absolute temperature difference between the process stream and the refrigerant. Must be greater than 2 F (1.1 K).

DUTy (H units/t units) =

Enter the desired enthalpy change of the process stream. Value must be negative.

SIMple

Simple exchanger (requires **U** & Area to be given). DESIGN II will determine the flow rate of the refrigerant such that it will vaporize from a bubble point liquid to a dew point vapor given the specified **U** and AREa.

U (U units) =

Overall heat transfer coefficient (default value is 50 BTU/HR/FT²/F)

AREa (L2 units) =

Heat transfer surface area per shell (default is 100 FT²)

NOTE: If the DUTy is specified, the process stream outlet temperature cannot approach the refrigerant temperature closer than 2 F (1.1 K). If the approach is less than 2 F it will be changed to a 10 F (5.56 K) temperature approach specification and the duty calculated.

Heat Exchanger: Air Cooled Heat Exchanger

The FIN FAN exchanger allows you to specify the AREa and **U** of the exchanger. This option would normally be used to simulate an existing air cooled heat exchanger where the area is known and the required air flow must be calculated. DESIGN II calculates the required flow, duty, corrected LMTD and outlet stream properties for the process stream. (enter all of the following)

FIN FAN

Air Cooled exchanger

TEMperature AIR IN (T units) =

Temperature of inlet air

TEMperature AIR OUT (T units) =

Temperature of outlet air

U (U units) =

Overall heat transfer coefficient (default is 50 BTU/HR/FT²/F)

AREa (L units) =

Heat transfer surface area per shell (default is 100 FT²)

Heat Exchanger Optional Command Details

Heat Exchanger: Basic Optional Commands

DELta pressure (P units) =

Enter pressure drop through the exchanger. For two inlet streams enter the pressure drop for the stream coded first, a comma, then the pressure drop for the second stream. Default is zero.

U (U units) =

Enter the overall heat transfer coefficient. Default is 50 BTU/HR/FT²/F (0.2839 KJ/SEC/M²/ K).

AREa (L2 units) =

Enter the area per shell for the SIMple exchanger specification or the WATER COOled exchanger option. Default is 100 FT² (9.29 M²).

SHELLs in PARallel =

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Enter the number of parallel shells. This command is ONLY valid for parallel shells when used in RATED heat exchangers. When no RATING is performed, this command is not used. Default is 1.

SHELLs in SERIES =

Enter the number of shells in series. This command is valid for series shells when used in non-RATED heat exchangers. When RATING is performed, the only configuration allowed is two E shells in which case it is 2 (see Figure 2 in [Heat Exchanger: Tube Commands](#)). Default is 1.

SHELL PASSES =

Enter the number of shell passes per shell. Default is 1. (First inlet stream coded is shellside.)

TUBE PASSES =

Enter the number of tube passes per shell. Default is 1. (Second inlet stream coded is tubeside.) If you have not already specified values for the number of SHELLs, SHELL PASSES, and TUBE PASSES, you should consider entering these commands. For type E shells, it is the total tube passes in the heat exchanger. Default values are one shell, one shell pass, and one tube pass.

NOTE: In Rating calculations for the AES and CHS exchanger types, SHE PAS = 1. For exchangers with an F shell (rating), SHE PAS = 2.

THFactor =

Enter this command to adjust the calculated tube side heat transfer coefficient by a factor. Default is 1.0

SHFactor =

Enter this command to adjust the calculated shell side heat transfer coefficient by a factor.

UFACTOR =

Enter this command to adjust the Overall Heat Transfer Coefficient.

NOTE: The **THF**, **SHF**, and **UFA** factor commands can be used individually or simultaneously as needed.

Heat Exchanger: Multiple Feed and Outlet Streams

Multiple feed streams can be specified on the shell and tube sides of the HEAt EXChanger. The shell side and tube side feeds will each be adiabatically flashed and mixed before HEAt EXChanger calculations are performed. Phase separation can be performed on heat exchanger product streams.

NUMBER of FEEDs 1 = Specify the number of shell side feeds

NUMBER of FEEDs 2 = Specify the number of tube side feeds

PRODUCT n = aaa Specify phase separation

where: n = 1 for the shell side product
n = 2 for the tube side product
aaa = SIN for single phase
aaa = TWO for two phase
aaa = THR for three phase

Heat Exchanger: Rating Commands

With the addition of a RATING command and appropriate commands for shell-and-tube geometry, DESIGN II will perform a rating calculation on any single phase counter-current exchanger and certain two-phase exchangers in your flowsheet. The commands are in the same, simple English-language format as other HEAt EXChanger commands. Most of the geometry commands have reasonable default values if you choose not to enter your own.

The module handles boiling or condensation occurring in either the shellside or the tubeside of a shell and tube heat exchanger; however, modeling of boiling in vertical shells is not allowed. If this configuration is specified, DESIGN II will default to a horizontal shell. Boiling in horizontal tubes is seldom required, but the program will perform the rating calculation for this geometry. No command is required to indicate a two-phase stream. Before the rating calculation is performed, DESIGN II automatically checks for vaporization or condensation in any of the streams and determines if a two-phase rating is required. Sample output is included in *Heat Exchanger Examples* No: 12 - 14.

Calculations

The rating calculations are performed for shell-and-tube exchangers. DESIGN II first performs the regular HEAt EXChanger calculation using the specifications you have entered to calculate outlet stream temperatures and total duty. All required properties for the rating calculation, such as viscosities, specific heats, thermal conductivities, densities, phase composition, and mass flows are automatically calculated for inlet and outlet conditions of both streams.

For 2-phase heat exchangers, the RATING option of the HEAt EXChanger module simulates the phase change along the longitudinal direction of the exchanger by dividing the exchanger into several sections.

In each section DESIGN II performs flashes and determines the two-phase flow regime. The module then chooses a heat transfer correlation that is best suited to the conditions and performs heat transfer and pressure drop calculations. Currently, the two-phase rating calculation accepts only two shell types: E and F, and the following exchanger configurations: 1-1, 1-2, 1-4, 2-2, 2-4, 2-6, 2-8. However, single phase rating is available for all shell types.

The only multiple shell heat exchanger configuration that can be rated in series is type E and only two shells may be specified.

The number of tube passes must be even. The normal configuration for two E shells in series would be counter current flow. For E shells in series, two additional commands are required:

INLet = SAME, TUBe FEEd = 2.

The rating calculation can be performed with or without a TEMperature OUT or DUTy specification. Without these specification (same as SIMple exchanger), DESIGN II performs a typical rating calculation determining the heat transferred and outlet temperatures based on inlet temperatures and heat exchanger configurations. Conversely, with a TEM OUT or DUTy specification, DESIGN II can estimate the area required to meet that specification.

The only true rating calculation DESIGN II performs is for the SIMple exchanger. Calculations performed with shell side specifications such as TEM OUT, DUTy, etc. cause DESIGN II to adjust the area. The program does not recalculate the velocity, delta pressure, or stream properties through the exchanger.

Any values entered for TUBe PASSes and/or SHEll PASSes will be used in both the regular HEAt EXChanger calculation and the rating calculation. TUB PAS and SHE PAS commands are used to correct the log mean temperature difference (LMTD) which is used in all counter-current calculations. The rating calculation uses these values for calculating total tube surface area and flow area. Values entered for U and AREa commands will be used for SIMple (and WAT COO or WAT COO CON) calculations; U will be used as an initial guess for the rating calculation. For the rating calculation, area is determined from the geometry. AREa should not be entered for a rating calculation. Either the KERN method or the BELL method can be chosen for the calculation of U and pressure drop (for both shell and tube).

The values for U, pressure drops, and area resulting from the rating calculation may differ significantly (which implies that a possible difference in calculated outlet temperatures) from the values you may have entered for the regular heat exchanger calculation.

NOTE: Default L units are feet.

RATe

You must enter this command to get a rating calculation.

U (U units) =

Enter the overall heat transfer coefficient. This value will be used as an initial guess. Default is 50 BTU/HR/FT²/ F (0.2839 KJ/SEC/M²/ K).

DELta pressure (P units) =

Enter maximum pressure drop through the exchanger. For two inlet streams enter the pressure drop for the stream coded first, a comma, then the pressure drop for the second stream. Default is zero.

NUMBER of INCrements =

Enter this command to specify the number of segments into which the exchanger is to be divided for the rating calculation. The accuracy of the rating is increased by increasing the number of increments. However, the rating will take longer to run and convergence will be more difficult to achieve as the number of increments are increased. The default is 5.

TOLerance =

Enter the heat exchanger rating convergence tolerance to be achieved. Default is 1E-06.

METHod for calculation =

Enter your choice for the U and pressure drop calculation for both the shell and tube sides. Options are **BELL** or **KERN**. Default is KERN.

EXChanger type =

Enter this command to specify the exchanger type. Choose one letter for front head, one letter for shell type, and one letter for rear head from standard T.E.M.A. nomenclature. Default is AEL.

A single phase rating calculation can be requested for shell-and-tube exchangers for any of the T.E.M.A. types. The two-phase rating calculation accepts only shell types E and F.

For the AES and CHS exchanger types, the number of shell passes is one. For multiple shells, enter a value for the SHElls in PARallel or SHElls in SERies command.

SHElls =

Enter the number of parallel shells. This command is ONLY valid for parallel (not series) shells when used in rated heat exchangers. When no RATing is performed, if the SHElls command is used then the exchanger is considered to be in series. Default is 1 for both rated and non-rated cases.

SINgle Phase

Enter command to perform single phase rating when both shell & tube side feed streams are considered to be single phase.

ENTrance factor =

Enter command for entrance/exit factor to include pressure losses on the tube side. Number of tube passes specified will be multiplied to estimate the overall tube side pressure drop. Default for ENTRance factor is zero.

SHElls in PARallel =

Enter the number of parallel shells. This command is ONLY valid for parallel shells when used in RATed heat exchangers. When no RATing is performed, this command is not used. Default is 1.

SHElls in SERies =

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Enter the number of shells in series. This command is valid for series shells when used in non-RATed heat exchangers. When RATING is performed, the only configuration allowed is two E shells in which case it is 2 (see Figure 2 in [Heat Exchanger: Tube Commands](#)). Default is 1.

CALculate **UCO**efficient

Use this option only for single phase stream exchangers. The single phase can be either all vapor or all liquid but not necessarily both vapor or liquid streams feeding to the same exchanger. If a stream is considered to be having two-phase flow then regular exchanger rating via vendor data is recommended. Default information given in the exchanger will be used for all parameters not specified. U coefficient will be used for the UA specification and temperature out specification. A single stream exchanger will work if the other stream is water which means that the stream must be coded within the simulation.

HORizontal or **VER**tical

This command specifies the shell orientation. Default is **HOR**izontal.

SHELL inside **DIAM**eter (L units) =

Enter the inside diameter of the shell. Default is 21.25 inches.

A fouling factor for the shell may be entered which will affect the value of the overall heat transfer coefficient.

SHELL FOUling factor (1/U units) =

Enter the shell fouling factor. Default is 0.0. Units allowed are 1/BTU/FT²/HR/ F, 1/KCAL/M²/HR/C, 1/KJ/M²/SEC/K, 1/CAL/M²/HR/C.

SHELL PASses =

Enter the number of shell passes per shell. Default is 1. (First inlet stream coded is shellside.)

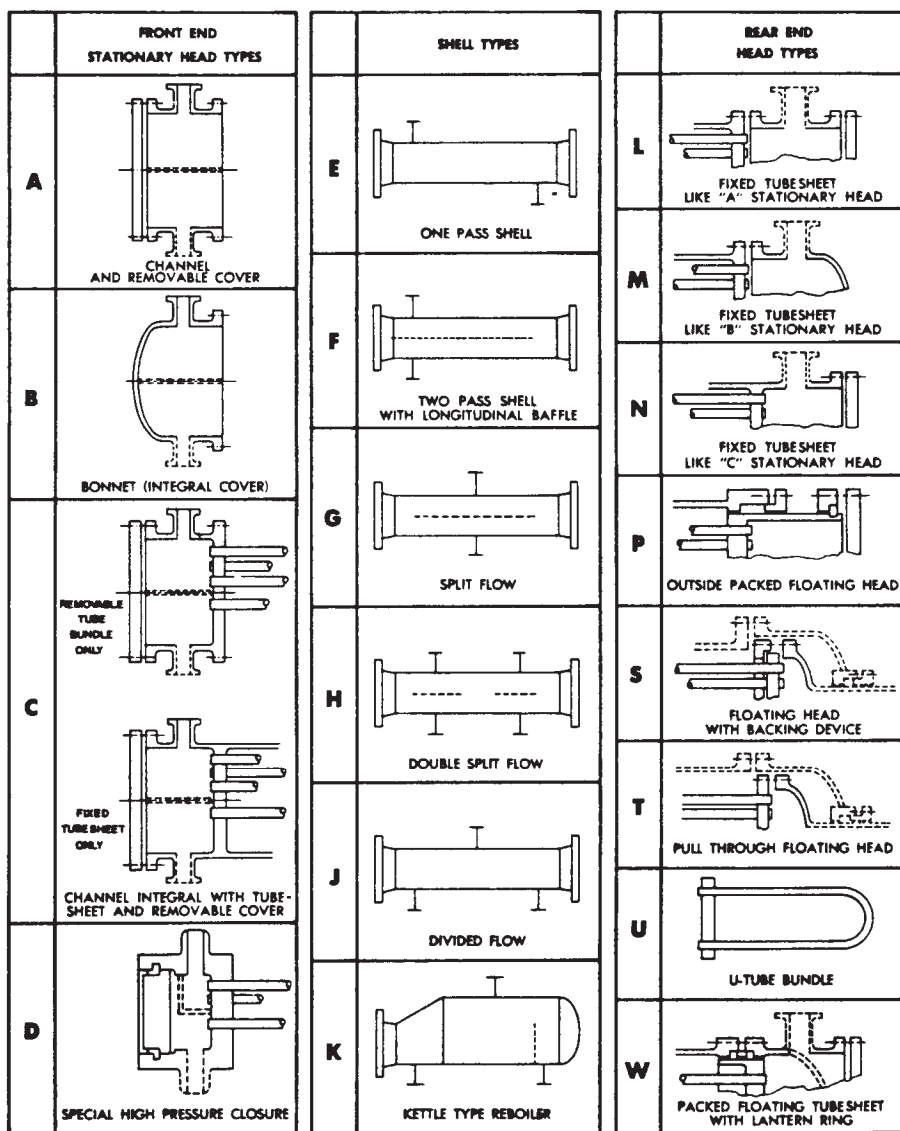


Figure 1 - T.E.M.A. Heat Exchanger Types

Heat Exchanger: Tube Commands

TUBside inlet **FLO**w direction =

This command is required only for a VERTical shell exchanger.

Enter **UP**ward or **DOWN**ward for the flow direction of the tubeside fluid. Default is UPward.

INLets =

Specify whether the tubeside inlet is located on the **SAM**e end of the shell as the shell inlet or on the **OPP**osite end. Default is OPP.

TUBe **FEE**d =

This command is required only when two shell passes are specified. **TUB**e **FEE**d = 1 feeds the tubeside fluid to the first shell pass.

or

TUBe **FEE**d = 2

feeds the tubeside fluid to the second shell pass. Default is 1.

Figure 2 - Possible 2-4 Heat Exchanger Configurations

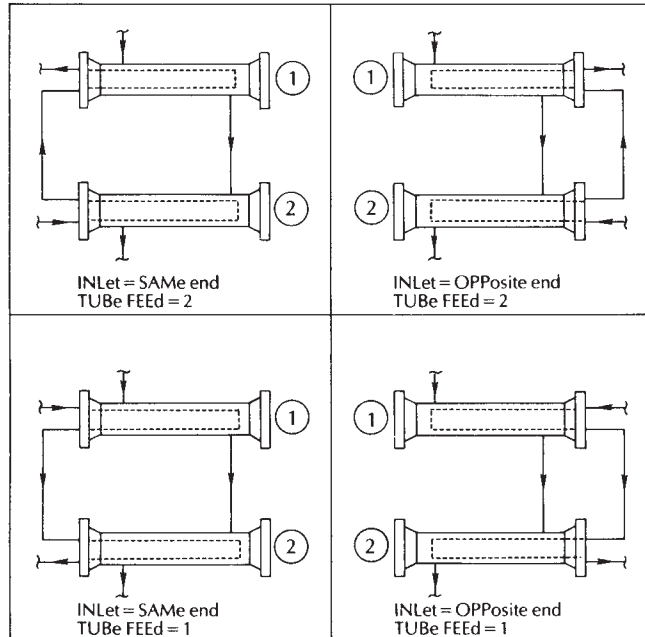
Figure 2 shows the four different configurations which may be used for a 2-4 heat exchanger.

Improved Convergence

Improvements have been made to the convergence methods to make the rating calculation more robust. The change is most notable in narrow boiling mixtures that undergo vaporization. The new methods improve modeling of pure components which undergo a phase change.

Rating of Heat Exchangers in Series

DESIGN II can rate two E shell heat exchangers in series. This configuration is shown below.



The commands to rate two E-shell exchangers in series are:

EXChanger type = xEx (where x represents the T.E.M.A. description for heat exchanger front and rear heads)

SHELL PASSes = 1

TUBE PASSes = n, where n is a number such as 1, 2, 3, or 4.

Note 1: The only multiple shell heat exchanger configuration that can be rated in series is a shell type E and only two shells may be specified.

Note 2: The normal configuration for two E shells in series would be counter current flow. This requires these additional commands:

INLet = SAME
TUBE FEEd = 2

Standard tube lengths are 8, 10, 12, 16, and 20 feet with 16 feet as the most common length. Sixteen feet is the default value if you do not enter a TUBE LENGTH command.

TUBE LENGTH (L units) =

Enter the length of the tubes. Default is 16 feet.

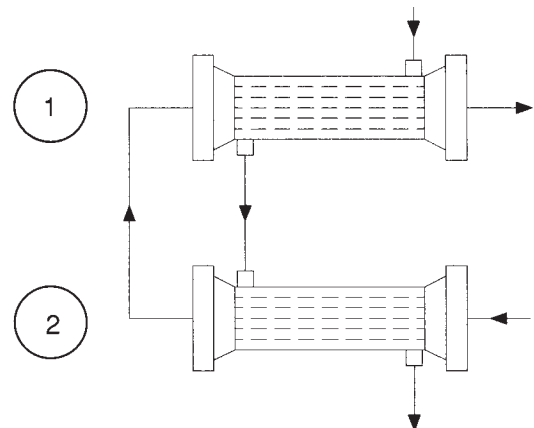
TUBE PITCH is defined as the shortest center-to-center distance between two adjacent tubes. The shortest distance between two tubes is called clearance. Tube pitch is normally in the range of 1.25 to 1.5 times the tube diameter. Clearance should not be less than one-fourth of the tube diameter and three-sixteenths of an inch is usually considered to be a minimum clearance.

TUBE PITCH (L units) =

Enter the tube pitch. Default is 0.9375 inches.

FIX tube PITCH

Adding this command will use the given TUBE PITCH to be applied even if it is less than the minimum clearance that is currently allowed per TUBE PITCH command above. However, the pitch is not allowed to be negative. A warning is printed



when this command is used, either to inform the user about the current pitch, or if the pitch is negative.

The TUBe BUNdle diameter command is only used in the Bell method for calculation of U and pressure drop for the shell side. If the command is not entered, a value will be calculated from the exchanger geometry.

TUBe BUNdle diameter (L units) =

Enter the diameter of the tube bundle. This command is only used for the Bell method. If no value is entered, it will be calculated from the geometry.

The TUBe FOULing factor, if specified, will be used in the calculation of the overall heat transfer coefficient.

TUBe FOULing factor =

Enter the fouling factor for the tubes. Default is 0.0. Allowable units are:

1/BTU/FT²/HR/F 1/KCAL/M²/HR/C 1/KJ/M²/SEC/K 1/CAL/M²/HR/C

TUBe PASSes is also used by the rating calculation. The default value for the number of TUBe PASSes is one. Entry of a value for this command affects both calculations.

TUBe PASSes =

Enter the number of tube passes per shell. Default is 1. (Second inlet stream coded is tubeside.)

NUMBER of TUBes =

Enter the number of tubes per shell pass. Default is 158.

Standard tube diameters range from 1/4-inch to 1-1/2 inch O.D. The most common diameters are 3/4-inch and 1-inch O.D. See *Heat Exchanger Tubing Characteristics Table*

TUBe INSide DIAMeter (L units) =

Enter the inside diameter of the tubes. If no value is entered, it will be calculated.

TUBe OUTside DIAMeter (L units) =

Enter the outside diameter of the tubes. Default is 0.75 inches.

TUBe BWG =

Enter the Birmingham Wire Gauge for tube wall thickness. Default is 16.

TUBe WALl thickness (L units) =

Enter the wall thickness of the tubes. If no value is entered, the program will calculate it.

Four commands describe the tube diameter/wall thickness. If you do not enter any of these commands, the default values of TUBe OUTside DIAMeter (IN) = 0.75 and TUBe WALl thickness (IN) = 0.065 which is equivalent to a BWG of 16 will be used. Any combination of the following commands (except for TUBe WALl thickness and TUBe BWG) can be entered:

- **TUBe WALl thickness**
- **TUBe INSide DIAMeter**
- **TUBe OUTside DIAMeter**
- **TUBe BWG**

If more than two of these commands are entered, the program will use the pair which is highest in the previous list. If only one of the above commands is entered, the following command will be used to complete the pair.

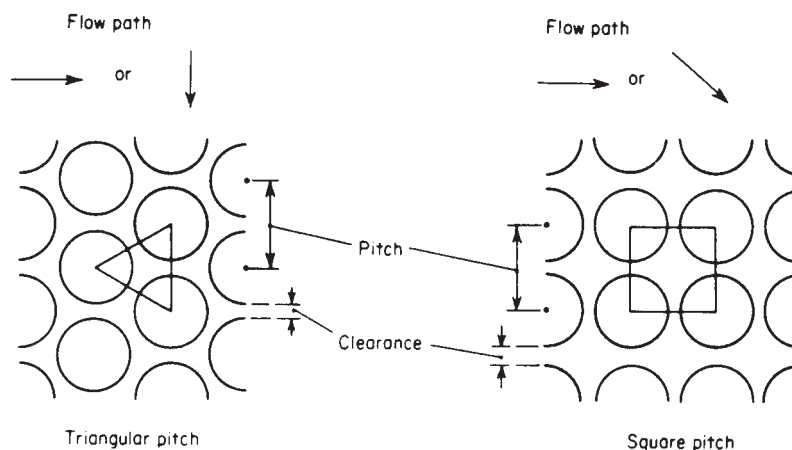
IF	THEN
TUB WAL	TUB OUT DIA(IN) = 0.75
TUB INS DIA	TUB WAL(IN) = 0.065
TUB OUT DIA	TUB WAL(IN) = 0.065
TUB BWG	TUB OUT DIA(IN) = 0.75

Tubes are normally laid out on a square or triangular pattern. The figure below illustrates the four available layout-flow path combinations. Square pitch has the advantage of easier external cleaning. Triangular pitch is sometimes preferred because the use of more tubes is permitted in a given shell diameter. See *Heat Exchanger: Standard Number of Tubes per Shell Table* for the number of tubes which can be placed in an exchanger with conventional tube sizes and layout.

TUBe LAYout =

Enter your choice for tube layout. Options are (Default is **SQU**are):

ROTated TRIangular	SQU are
ROTated SQU are	TRIangular



If you cannot find the specific tube material in the *Tube Metallurgy Table*, enter the keyword for the material which has an average thermal conductivity closest to the desired material.

TUBE MATERIAL =

Enter choice of tube material. (default is **CARbon steel**):

ADMiralty brass
ALLOy 225
CARbon steel
CARbon **MOLy** Steel
STAINless steel **214**
STAINless steel 304
ALUminum
MONel
RED brass
COPper
COPper nickel **90/10**
COPper nickel **70/30**
NICKel
TITanium

Also, see *Tubing Characteristics Table*, *Standard Number of Tubes per Shell Table*, *Tube Metallurgy Table*.

Heat Exchanger: Tubing Characteristics Table

Tubing O.D. in	BWG gage	Wall thickness in	Inside cross sectional area in ²	Sq. ft external sectional per ft length	Sq. ft internal surface per ft length	Weight per ft length steel lbs	Tubing I.D. in
1/4	22	.028	.0296	.0654	.0508	.066	.194
1/4	24	.022	.0333	.0654	.0539	.054	.206
1/4	26	.018	.0360	.0654	.0560	.044	.214
3/8	18	.049	.0603	.0982	.0725	.171	.277
3/8	20	.035	.0731	.0982	.0798	.127	.305
3/8	22	.028	.0799	.0982	.0835	.104	.319
3/8	24	.022	.0860	.0982	.0867	.083	.331
1/2	16	.065	.1075	.1309	.0969	.302	.370
1/2	18	.049	.1269	.1309	.1052	.236	.402
1/2	20	.035	.1452	.1309	.1126	.174	.430
1/2	22	.028	.1548	.1309	.1162	.141	.444
5/8	12	.109	.1301	.1636	.1066	.602	.407
5/8	13	.095	.1486	.1636	.1139	.537	.435
5/8	14	.083	.1655	.1636	.1202	.479	.459
5/8	15	.072	.1817	.1636	.1259	.425	.481
5/8	16	.065	.1924	.1636	.1296	.388	.495
5/8	17	.058	.2035	.1636	.1333	.350	.509
5/8	18	.049	.2181	.1636	.1380	.303	.527
5/8	19	.042	.2299	.1636	.1416	.262	.541
5/8	20	.035	.2419	.1636	.1453	.221	.555
3/4	10	.134	.1825	.1963	.1262	.884	.482
3/4	11	.120	.2043	.1963	.1335	.809	.510

3/4	12	.109	.2223	.1963	.1393	.748	.532
3/4	13	.095	.2463	.1963	.1466	.666	.560
3/4	14	.083	.2679	.1963	.1529	.592	.584
3/4	15	.072	.2884	.1963	.1587	.520	.606
3/4	16	.065	.3019	.1963	.1623	.476	.620
3/4	17	.058	.3157	.1963	.1660	.428	.634
3/4	18	.049	.3339	.1963	.1707	.367	.652
3/4	20	.035	.3632	.1963	.1780	.269	.680
7/8	10	.134	.2894	.2291	.1589	1.061	.607
7/8	11	.120	.3167	.2291	.1662	.969	.635
7/8	12	.109	.3390	.2291	.1720	.891	.657
7/8	13	.095	.3685	.2291	.1793	.792	.685
7/8	14	.083	.3948	.2291	.1856	.704	.709
7/8	16	.065	.4359	.2291	.1950	.561	.745
7/8	18	.049	.4742	.2291	.2034	.432	.777
7/8	20	.035	.5090	.2291	.2107	.313	.805
1	8	.165	.3526	.2618	.1754	1.462	.670
1	10	.134	.4208	.2618	.1916	1.237	.732
1	11	.120	.4536	.2618	.1990	1.129	.760
1	12	.109	.4803	.2618	.2047	1.037	.782
1	13	.095	.5153	.2618	.2121	.918	.810
1	14	.083	.5463	.2618	.2183	.813	.834
1	15	.072	.5755	.2618	.2241	.714	.856
1	16	.065	.5945	.2618	.2278	.649	.870
1	18	.049	.6390	.2618	.2361	.496	.902
1	20	.035	.6793	.2618	.2435	.360	.930
1 1/4	7	.180	.6221	.3272	.2330	2.057	.890
1 1/4	8	.165	.6648	.3272	.2409	1.921	.920
1 1/4	10	.134	.7574	.3272	.2571	1.598	.982
1 1/4	11	.120	.8012	.3272	.2644	1.448	1.010
1 1/4	12	.109	.8365	.3272	.2702	1.329	1.032
1 1/4	13	.095	.8825	.3272	.2775	1.173	1.060
1 1/4	14	.083	.9229	.3272	.2838	1.033	1.084
1 1/4	16	.065	.9852	.3272	.2932	.823	1.120
1 1/4	18	.049	1.0423	.3272	.3016	.629	1.152
1 1/4	20	.035	1.0936	.3272	.3089	.456	1.180
1 1/2	10	.134	1.1921	.3927	.3225	1.955	1.232
1 1/2	12	.109	1.2908	.3927	.3356	1.618	1.282
1 1/2	14	.083	1.3977	.3927	.3492	1.258	1.334
1 1/2	16	.065	1.4741	.3927	.3587	.996	1.370
2	11	.120	2.4328	.5236	.4608	2.410	1.760
2	13	.095	2.5730	.5236	.4739	1.934	1.810
2 1/2	9	.148	3.8152	.6545	.5770	3.719	2.204

Heat Exchanger: Standard Number of Tubes per Shell Table

Table 2						
ONE-PASS		TWO-PASS			FOUR-PASS	
Shell I.D. in	Square pitch	Triangular pitch	Square pitch	Triangular pitch	Square pitch	Triangular pitch
3/4-inch OD tubes on 1-inch pitch						
8	32	37	26	30	20	24
12	81	92	76	82	68	76
15.25	137	151	124	138	116	122
21.25	277	316	270	302	246	278
25	413	470	394	452	370	422
31	657	745	640	728	600	678
37	934	1074	914	1044	886	1012

1 inch OD tubes on 1 1/4-inch pitch

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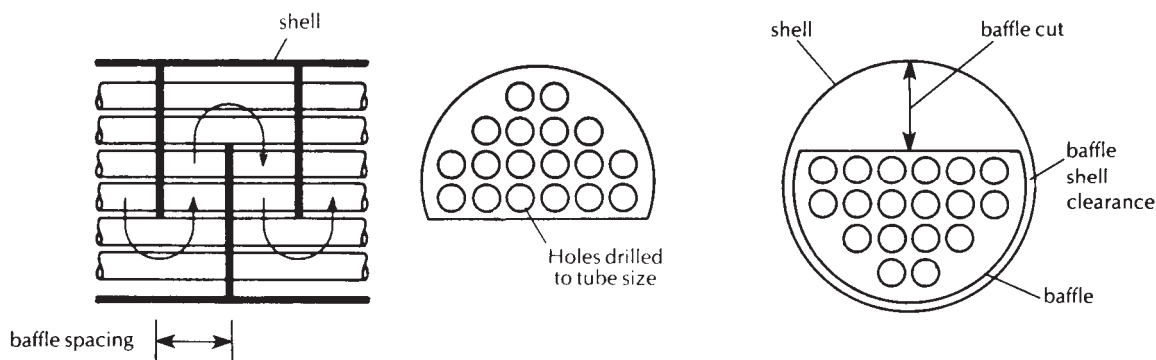
8	21	21	16	16	14	16
12	48	55	45	52	40	48
15.25	81	91	76	86	68	80
21.25	177	199	166	188	158	170
25	260	294	252	282	238	256
31	406	472	398	454	380	430
37	596	674	574	664	562	63

Heat Exchanger: Tube Metallurgy Table

Material	Average Thermal Conductivity (BTU/FT/HR/F)
Keyword in bold	
ADM iralty brass	70.00
ALU minum	109.00
ALLO y 825	8.10
CAR bon steel	26.00
CAR bon MOL y steel	25.00
COP per	225.00
COP per nickel 90/10	41.00
COP per nickel 70/30	17.00
MON el	15.00
NICK el 200	35.00
RED brass	92.00
STAIN less steel 304	10.00
STAIN less 214	21.00
TITAN ium	11.50
PVC	0.10
GLASS	0.6667

Heat Exchanger: Baffle Commands

Although the presence of baffles in the shell side increases the pressure drop on the shell side, the advantage of better mixing of the fluid and increased turbulence more than offsets the pressure drop disadvantage. The distance between baffles is known as BAFfle SPACing. In general, baffle spacing is never greater than a distance equal to the diameter of the shell or less than one-fifth of the shell diameter. The most common type of baffle used in heat exchangers is the segmented baffle. This is the type of baffle the rating calculation models. Many segmented baffles have a baffle height that is 75 percent of the inside diameter of the shell. This would correspond to an entry of BAFfLE CUT=0.25. See Figure 4 for details. Disk and doughnut or orifice baffles are not currently modeled.



BAFfle SPACing (L units) =

Enter the baffle spacing. Default is 5 inches.

BAFfle CUT =

Enter the fractional value for the baffle cut. The value must be between 0.0 and 0.49. Default is 0.2.

The BAFfle shell CLearance can be specified for use in the Bell method for U and shell pressure drop calculation. If no value is entered, the program will calculate one from the exchanger geometry.

BAFfle shell CLearance (L units) =

Enter the clearance between the shell and baffles. This command is only used with the Bell method. If no value is specified, it will be calculated from the geometry.

Sealing strips are added to baffles to prevent bypass leakage. Enter a value for the NUMber of SEAling strips if your exchanger has more than two. This value is only for inclusion in the printout and is not used in the rating calculation.

NUMber of SEAling strips =

Enter the number of sealing strips for baffles. Default is 2.

Heat Exchanger: Additional Output Commands

The GENeral section also has HEating CURve and COOLing CURve commands which can be used on any stream in the flowsheet. Heating or cooling curve information, shown below, can be obtained for a heat exchanger by specifying the following command types:

COMMAND 1:

CURve INCrements =

Enter the number of increments for heating curves.

Example:

```
HEAT EXCHANGER IN CONDENSING CURVE MODE
NUMBER OF TEMPERATURE INCREMENTS ON STREAM 1 = 4
EQUIPMENT NUMBER = 1
FOLLOWING CALCULATIONS BASED ON END POINT OF HEAT EXCHANGER
TOTAL HEAT TRANSFERRED FROM STREAM 1, BTU/HR .38010E 07 AREA = 2764.7 FT2 CORRECTED LOG MEAN TEMP. =
27.50 DEG F
MOL. WT. STREAM 1 = 20.50 MOL. WT. STREAM 2 = 17.01
FOLLOWING CALCULATIONS ARE FOR HEAT EXCHANGER DIVIDED INTO INCREMENTS
```

INC	TEMP	VAPOR	TEMP	VAPOR	CHANGE	AREA	LMTD
NO	DEG F	FRAC	DEG F	FRAC	BTU/HR	FT2	DEG F
0	-58.6	.6559	-127.9	.9971	.00000	0.0	0.0
1	-17.7	.8452	-56.1	1.0000	.12683E07	485.0	52.3
2	23.2	.9578	9.2	1.0000	.10662E07	883.0	24.2
3	64.1	.9996	60.0	1.0000	.83240E06	2073	8.0
4	105.0	1.0000	98.2	1.0000	.63411E07	2393	5.3

```
TOTAL AREA FOR 4 DIVISIONS IN THIS HXER = 5833.8 FT2
TOTAL HEAT TRANSFERRED = .39010+07 BTU/HR
```

Heat exchanger curves should be done as a separate run since the curve information requires a significant additional amount of time. By running heat exchanger curves in a separate run, you can be sure your process design is correct before spending time in final design information.

NOTE: The geometry of the exchanger for CUR INC output is based on one shell, one tube pass, one shell pass, regardless of the geometry commands entered for the heat exchanger. Stream 1 refers to the first inlet stream and stream 2 is the second inlet (tubeside).

COMMAND 2:

Q-T

Enter this command to have duty versus temperature curves plotted for heat exchangers.

The Q-T table and plot are useful tools for evaluating exchanger design. These curves are based on end-point temperature results. You can quickly determine the minimum temperature approach or locate regions with unrealistically high $U \times A$ or temperature crossovers. In addition, bubble points and dew points are marked when vaporization or condensation occurs for either hot or cold streams.

To get this additional report, add the command: **Q-T**

This command can be used in conjunction with HEAt EXChanger RATing.

NOTE: Use of the CURve INCrements command is not allowed with the Q-T command.

When using the **Q-T** command, the following print option may be useful.

COMMAND 3:

MINimum TEMperature APProach (T units) =

Used only with the Q-T command. Enter a minimum temperature of approach value. The first point where the approach temperature falls below this value will be marked with the label MN in the Q-T tabular output. Default is 10 F.

Sample output for the Q-T print option can be found in the LNG Exchanger Example 6 - *LNG Exchanger: Q-T Diagram*.

COMMAND 4:

TEMperature of EXChange (T units) =

Enter value for exchange temperature for the utility side of the exchanger (for single stream exchangers only). Default temperatures are 250 F for heating fluids, 70.3 F for cooling fluids. This command is used only in conjunction with the LOST work command which is entered in the GENeral section.

Heat Exchanger: Thermodynamic Commands

Use these commands to specify options for the module only when they are different than the system thermodynamics specified in the GENeral commands. Options are given in Thermodynamics Section.

HKEy =

Enter symbolic name of enthalpy option. (e.g. HKE = GRA)

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KKEY =

Enter symbolic name of K-value option. (e.g. **KKE = ESSOK**)

DKEY =

Enter symbolic name of density option. (e.g. **DKE = IDEALD**)

LIQUID DKEY =

Enter symbolic name for liquid density option.(e.g. **LIQUID DKEY = PEND**)

VSVKEY =

Enter symbolic name for vapor viscosity. (e.g. **VSVKEY = DEAN**)

VSLKEY =

Enter symbolic name for liquid viscosity. (e.g. **VSLKEY = API**)

THVKEY =

Enter symbolic name for vapor thermal conductivity. (e.g. **THVKEY = NBS81**)

THLKEY =

Enter symbolic name for liquid thermal conductivity. (e.g. **THLKEY = TEMA**)

STKEY =

Enter symbolic name for surface tension. (e.g. **STKEY = API**)

The commands above specify the thermodynamics for shell side streams of counter-current (two-stream) exchangers. To specify different thermodynamics for the tubeside stream only, the following commands may be used.

HKEY 2 =

Enter symbolic name of enthalpy option for tubeside stream. (e.g. **HKE 2= GRA**)

KKEY 2 =

Enter symbolic name of K-value option for tubeside stream. (e.g. **KKE 2= ESSOK**)

DKEY 2 =

Enter symbolic name of density option for tubeside stream. (e.g. **DKE 2= IDEALD**)

LIQUID DKEY 2 =

Enter symbolic name for liquid density option.(e.g. **LIQUID DKEY 2 = PEND**)

VSVKEY 2 =

Enter symbolic name for vapor viscosity for tube side stream.. (e.g. **VSVKEY 2 = DEAN**)

VSLKEY 2 =

Enter symbolic name for liquid viscosity for tube side stream.. (e.g. **VSLKEY 2 = API**)

Heat Exchanger: Output Control

- Temperature profile plots for E and F shell type single phase and two-phase rating calculations are plotted automatically
- Rating table and temperature profile plots appear in the equipment summary. This information can be printed in the NOW CALLING section by using the following two heat exchanger commands:
- **PRInt RATing**
- **PLOt ON**

Heat Exchanger Command Summary

Single Stream Exchanger Commands

TEM OUT (T units) =

DUTy (H units/t units) =

TEMperature OUT is **BUB**ble point

TEMperature OUT is **DEW** point

DELta TEMperature (T units) =

Single Stream Exchanger Optional Commands

TEMperature of **WATER IN** (T units) =

TEMperature of **WATER OUT** (T units)

Counter-Current Heat Exchangers Commands

SIMple exchanger

AREa (L2 units) =

TEMperature **APP**roach (T units) =

TEMperature **OUT** Shell Side (T units) =

TEMperature **OUT TUB**e Side (T units) =

DUTy (H units/t units) =

Shell Side **TEM**perature **OUT** is **BUB**ble point

Shell Side **TEM**perature **OUT** is **DEW** point

Optional Commands

TEMperature of **EX**Change (T units) =

CURve **INC**rements =

DELta pressure (P units) =

U (U units) =

AREa (L2 unit) =

SHElls =

SHEll **PAS**ses =

TUBe **PAS**ses =

THFactor =

SHFactor =

UFactor =

Thermo option for shellside and tubeside streams (two & single-stream exchanger)

HKEY =

KKEY =

DKEY =

LIQUID DKEY =

Shell Side **DEL**ta **TEM**perature (T units) =

Counter-Current Exchanger Optional Commands

U (U units) =

Water-Cooled Exchanger Commands

WATER COOled exchanger

WATER COOled **COND**enser

TEMperature of **WATER IN** (T units) =

TEMperature of **WATER OUT** (T units) =

AREa (L2 units) =

Refrigerant Exchanger Commands

REFR = **TUBE** or **SHELL**

PREssure of **REF**rigerant (P units) i =

TEMperature of **REF**rigerant (T units) i =

Shell Side **DEL**ta **TEM**perature (T units) =

TEMperature **OUT** Shell Side (T units) =

TEMperature **APP**roach (T units) =

DUTy (H units/t units) =

Baffle Commands

BAFfile **SPA**cing (L units) =

BAFfile **CUT** =

BAFfile shell **CLE**arance (L units) =

NUMber of **SEA**ling strips =

Additional Output Commands

CURve **INC**rements =

Q-T

MIN TEM APP (T units) =

Thermo for tubeside stream only

HKEy 2 =

KKEy 2 =

DKEy 2 =

Water Immiscibility

IMM = 62

NO IMM

VSVKEY =

VSLKEY =

THVKEY =

THLKEY =

STKEY =

Thermo for tubeside stream only (two-stream exchanger only)

HKEy 2 =

KKEy 2 =

DKEy 2 =

LIQuid **DKEy 2** =

VSVKEY 2 =

VSLKEY 2 =

THVKEY 2 =

THLKEY 2 =

STKEY 2 =

Heat Exchanger Rating Commands

RATE

AREa (L2 units) =

U (U units) =

DELta pressure (P units) =

NUMber of **INC**rements =

TOLerance =

MINimum **TEM**perature of approach (T units) =

METHod for calculation =

EXchanger type =

SHELls =

HORizontal or **VER**tical

SHELl inside **DIA**meter (L units) =

SHELl **FOU**ling factor =

SHELl **PAS**ses =

TUBeside inlet **FLO**w direction =

INLets =

TUBe **FEE**d

TUBe **LEN**gth (L units) =

TUBe **PIT**ch (L units) =

TUBe **BUN**dle diameter (L units) =

TUBe **FOU**ling factor =

TUBe **PAS**ses =

NUMber of **TUB**es =

TUBe **INS**ide **DIA**meter (L units) =

TUBe **OUT**side **DIA**meter (L units) =

TUBe **BWG** =

TUBe **WAL**l thickness (L units) =

TUBe **LAY**out =

TUBe **MAT**erial =

Heat Exchanger Step by Step

Heat Exchanger STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet stream(s)

HEA EXC

Assigned equipment flowsheet number

User choice - up to 16 characters

One or two

One or two - must match number of inlet streams

NOTE: The 1st inlet stream coded becomes 1st outlet stream coded and the 2nd inlet stream coded becomes the 2nd outlet stream coded.

Heat Exchanger STEP 2

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Choose a heat exchanger type. Select ONE of the following heat exchanger types.

- Single stream; code with one inlet stream and one outlet stream
 - only one side of the exchanger is involved
 - program will calculate the outlet temperature and/or duty
- Counter-current; code with two inlet streams and two outlet streams
 - first inlet stream coded will be shell side inlet
- Water cooled exchanger; code with one inlet stream and one outlet stream
 - program will calculate process outlet temperature and water flowrate based on specified (or default) U and AREa
 - process stream is assumed to be on the shell side
 - water stream is not coded as an inlet or outlet stream
- Water cooled condenser; code with one inlet stream and one outlet stream
 - program will calculate process outlet temperature set to the bubble point and will calculate water flowrate, duty and area
 - process stream is assumed to be on the shell side
 - water stream is not coded as an inlet or outlet stream
- Refrigerant; code with two inlet streams and two outlet streams
 - program will calculate process stream outlet temperature or duty and then calculate refrigerant flow rate at a specified temperature and pressure
 - only a single component refrigerant may be used
 - refrigerant enters the exchanger at the bubble point and leaves at the dew point
 - the refrigerant must be coded as the second inlet and outlet, refrigerant component ID number must be in the COMponent list (refrigerant outlet flow is calculated; no inlet flow is used)
 - process stream must be coded as first inlet stream and will be on the shell side

Heat Exchanger STEP 3

Enter the required specifications and desired options for the selected heat exchanger type.

Single stream exchanger (enter ONE of the following).

Temperature of the outlet stream
Enthalpy change (- for cooling, + for heating) of the stream
Set temperature of outlet stream to the bubble point
Set temperature of outlet stream to the dew point
Temperature change from inlet to outlet (positive value indicates heating;
negative value indicates cooling)

TEM OUT (T units) =
DUT (H units/t units) =
TEM OUT BUB
TEM OUT DEW
DEL TEM (T units) =

Optional commands (enter any of the following options)

Inlet cooling water temperature (default is 90 F)
Outlet cooling water temperature (default is TEM WAT IN plus 15 F)

TEM WAT IN (T units) =
TEM WAT OUT (T units) =

Counter-current exchanger (enter ONE of the following)

IF simple exchanger enter **ALL** of the following specifications

Simple exchanger
Heat transfer surface area per shell (stream outlet temperature is calculated from specified AREa and U; default is 100 FT²)
Overall heat transfer coefficient default is 50 BTU/HR/FT²/ F
Absolute temperature difference between stream coded as the first outlet stream and stream coded as the second input stream (must be greater than 2 F)
Temperature of stream coded as the first outlet stream (will correspond to the stream coded as the first inlet stream). This is for shell side outlet stream.
Temperature out of tube side
Enthalpy change (- for cooling, + for heating) of the stream coded as the first inlet stream
Set temperature of stream coded as the first outlet stream to the bubble point. This is for shell side outlet stream.
Set temperature of stream coded as the first outlet stream to the dew point. This is for shell side outlet stream.
Temperature change from inlet to outlet (+ value indicates heating; - value indicates cooling). This is for shell side outlet stream.

SIM
ARE (L units) =

U (U units) =
TEM APP (T units) =

TEM OUT (T units) =

TEM OUT TUB (T units) =
DUT (H units/t units) =

TEM OUT BUB

TEM OUT DEW

DEL TEM (T units) =

Water cooled exchanger (enter ALL of the following)

Water cooled exchanger
Overall heat transfer coefficient (default is 50 BTU/HR/FT²/ F)
Heat transfer surface area per shell (default is 100 FT²)
Inlet cooling water temperature (default is TEM WAT IN plus 15 F)

WAT COO
U (U units) =
ARE (L units) =
TEM WAT OUT (T units) =

Water cooled condenser (enter ALL of the following)

Water cooled condenser

WAT COO CON

Inlet cooling water temperature (default is 90 F)	TEM WAT IN (T units) =
Outlet cooling water temperature (default is TEM WAT IN plus 15 F)	TEM WAT OUT (T units) =
Refrigerant exchanger (enter the following specifications)	
• Enter ONE of the following refrigerant specifications	
Pressure at which the refrigerant temperature is to be calculated (the "I" refers to the component ID number, not the refrigerant stream number)	PRE REF (P units) i =
Temperature of the refrigerant (the "I" refers to component ID number, not the refrigerant stream number)	TEM REF (T units) i =
• Enter ONE of the following four process stream specifications	
Temperature change from inlet to outlet (- for cooling, + for heating). This is shell side outlet stream.	DEL TEM (t UNITS) =
Outlet temperature of process stream on shell side	TEM OUT (T units) =
Absolute temperature difference between process stream and the refrigerant (MUST be greater than 2 F)	TEM APP (T units) =
Enthalpy change of the process stream (- for cooling, + for heating)	DUT (H units/t units) =

Heat Exchanger STEP 4

Choose any of the optional heat exchanger specifications below.

Select any of the following options.

Pressure drop through the exchanger (for two inlet streams enter the pressure drops for the first and second streams separated by commas; default is zero)	DEL (P units) =
Overall heat transfer coefficient (if U and AREa are not required commands, the AREa is calculated as $AREa = Q/U \cdot LMTD$); default is 50 BTU/HR/FT ² / F)	U (U units) =
Heat transfer surface area per shell (default is 100 FT ²)	ARE (L2 units) =
Number of parallel shells (default is 1)	SHE =
Number of shell passes per shell (default is 1)	SHE PASS =
Number of tube passes per shell (default is 1)	TUB PASS =
Adjust the calculated tube side heat transfer coefficient by a factor. Default is 1.0	THF =
Adjust the calculated shell side heat transfer coefficient by a factor	SHF =
Adjust the overall heat transfer coefficient	UFA =

Heat Exchanger STEP 5

Enter the required specifications and options for heat exchanger rating.

Heat exchanger rating (enter the following required command).

Heat exchanger rating

RAT

- Effect of specifications on **RAT**ing calculations

- IF a SIMPLE or water cooled exchanger/condenser is specified THEN outlet temperatures will be calculated from exchanger area and heat transfer coefficients.

- IF any other exchanger types, THEN outlet stream temperatures are calculated first followed by the AREa needed to meet the outlet temperatures.

Heat exchanger rating options (select any of the following)

Heat transfer area per shell (will override area calculated from geometry) **ARE** (L2 units) =

- this command should not be entered for RATing. RATing should use AREa as defined from geometry or delta pressure, velocity, etc. will not be consistent.

Overall heat transfer coefficient (used for initial guess only and will be ignored for rating calculation; default is 50 BTU/HR/FT²/ F) **U** (U units) =

Pressure drop through the exchanger (for two inlet streams enter the pressure drops for the first and second streams separated by commas; will be used as maximum allowable pressure drop only for two-phase calculations for rating purposes; single-phase calculations pressure drop calculation are not check for maximum delta pressure) **DEL** (P units) =

Number of exchanger calculation segments (default is 5) **NUM INC** =

Enter the heat exchanger rating convergence tolerance to be achieved. Default is 1E-06. **TOL** =

Minimum temperature approach between shell and tube (default is 10 F) **MIN TEM** (T units) =

Heat exchanger rating calculation method (enter ONE of the following)

Kern method (default)

MET = KERN

Bell method

MET = BELL

Heat Exchanger STEP 6

Enter the required specification to identify exchanger type. Exchanger type specification (see reference for options).

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Enter the three TEMA letter code for exchanger type (only shell types E and F are available for two phase heat exchanger rating; default is AEL)

EXC =

Heat Exchanger STEP 7

Enter the required specifications to identify shell geometry.

Shell specifications (enter ALL of the following)

Number of parallel shells (**ALL** following specifications and options will apply to number of shells specified here; default is 1)

SHE =

Shell orientation (enter **ONE** of the following options)

horizontal shell (default)

vertical shell (calculations will default to horizontal if shell side is two phase)

Shell inside diameter (default is 21.25 IN)

Shell fouling factor (default is 0.0)

Number of shell passes (default is 1)

HOR

VER

SHE DIA (L units) =

SHE FOU =

SHE PAS =

Heat Exchanger STEP 8

Enter the required specifications to identify tube geometry. (enter ALL of the following)

- Inlet specification (enter **ONE** of the following)

tubeside inlet located on opposite end of shell as the shell inlet (default)

tubeside inlet located on same end of shell as the shell inlet

INL = OPP

INL = SAM

- Tubeside flow direction (enter only if shell is VERTICAL; select **ONE** of the following)

upward tubeside flow direction (default)

downward tubeside flow direction

TUB FLO = UP

TUB FLO = DOWN

- Tube feed specification (enter only if SHE PAS = 2; select **ONE** of the following)

tubeside inlet to first shell pass (default)

tubeside inlet to the second shell pass

Tube length (default is 16 FT)

Tube pitch (default is 0.9375 IN)

Tube bundle diameter (used if Bell method selected; program will calculate if not defined)

Tube fouling factor (default is 0.0)

Number of tube passes (default is 1)

Number of tubes (default is 158)

TUB FEE = 1

TUB FEE = 2

TUB LEN (L units) =

TUB PIT (L units) =

TUB BUN (L units) =

TUB FOU =

TUB PAS =

NUM TUB =

- Tube wall thickness and diameter specifications (enter **UP TO TWO** options)

tube inside diameter (default is calculated)

tube outside diameter (default is 0.75 IN)

- IF tube wall thickness THEN select **ONE** of the following (default is 16 BWG)

+ Birmingham wire gauge

+ Tube wall thickness

TUB INS DIA (L units) =

TUB OUT DIA (L units) =

TUB BWG =

TUB WAL (L units) =

- Tube sheet layout specification (enter **ONE** of the following)

square (default)

rotated square

Triangle

rotated triangle

TUB LAY = SQU

TUB LAY = ROT SQU

TUB LAY = TRI

TUB LAY = ROT TRI

- Tube material specification (enter **ONE** of the following)

Carbon steel (default)

Carbon Moly steel

Admiralty brass

Alloy 225

Stainless steel 214

Stainless steel 304

Monel

Red brass

Copper nickel 90/10

Copper nickel 70/30

Nickel

Titanium

TUB MAT = CAR

TUB MAT = CAR MOL

TUB MAT = ADM

TUB MAT = ALL 225

TUB MAT = STA 214

TUB MAT = STA

TUB MAT = MON

TUB MAT = COP

TUB MAT = COP 90

TUB MAT = COP 70

TUB MAT = NIC

TUB MAT = TIT

Heat Exchanger STEP 9

Enter the required specifications to identify baffle geometry. Baffle specifications (enter ALL of the following)

Baffle spacing (default is 5 IN)

Baffle cut fractional value (default is 0.2 maximum is 0.49)

BAF SPA (L units) =

BAF CUT = fraction

Baffle shell clearance (used if Bell method selected; program will calculate if not defined)
 Number of sealing strips (default is 2)

BAF CLE (L units) =
NUM SEA =

Heat Exchanger STEP 10

Choose any of the additional options below. Additional output information (select ONE of the following).

Number of increments for heating/cooling curves, not allowed if the Q-T command is used (default is no curve)
 Duty-temperature curve (default is no curve)
 Minimum approach temperature (marks tabular output with the label "MN" at point of specified minimum approach)

CUR INC =

Q-T

MIN TEM APP (T units) =

Select ANY of the following options

Value for exchange temperature for the utility side of the exchanger (only used for single stream exchanger; default temperatures are 250 F for heating fluids, 70.3 F for cooling fluids)

TEM EXC (T units) =

This command is used only in conjunction with the LOST work command which is entered in the GENeral section.

If thermo is different from global (GENeral section) options THEN select the commands below. If specified, they will apply to shellside stream.

K-value option
 Enthalpy option
 Density option
 Enter symbolic name for vapor viscosity.
 Enter symbolic name for liquid viscosity.
 Enter symbolic name for vapor thermal conductivity.
 Enter symbolic name for liquid thermal conductivity.
 Enter symbolic name for surface tension.

KKE =

HKE =

DKE =

VSVKEY =

VSLKEY =

THVKEY =

THLKEY =

STKEY =

To specify different thermo for tubeside stream only (counter-current only) select

K-value option for tubeside stream
 Enthalpy option for tubeside stream
 Density option for tubeside stream
 Enter symbolic name for vapor viscosity for tube side stream.
 Enter symbolic name for liquid viscosity for tube side stream.
 Enter symbolic name for vapor thermal conductivity for tube side stream.
 Enter symbolic name for liquid thermal conductivity for tube side stream.
 Enter symbolic name for surface tension for tube side stream.

KKE2 =

HKE2 =

DKE2 =

VSVKEY 2 =

VSLKEY 2 =

THVKEY 2 =

THLKEY 2 =

STKEY 2 =

Heat Exchanger Examples

There are several sample flowsheets in "Chapter 25: Heat Exchanger Samples - c:\designii\samples\equipmnt\heaexc" of the DESIGN II for Windows Tutorial and Samples Guide.

Heat Exchanger: Specifying Multiple Feed and Outlet Streams

AB123.

* HEAT EXCHANGER PHASE SEPARATION

C- The following example illustrates how to specify two shell side

C- feeds and one tube side feed with phase separation of the shell c- side products.

HEAt EXChanger 3 = E301,1,2,3,-4,-5,-6,

TEM OUT (F) = 115

DEL (PSIA) = 7

NUM FEE 1 = 2

NUM FEE 2 = 1

Product 1 = TWO

Heat Exchanger References

- Bell, K.J., "Exchanger Design", *Petro/Chem Engineer*, p. C-26, October, 1960.
- Kern, D.G., *Process Heat Transfer*, McGraw-Hill Book Co., Inc. New York, N.Y., 1950.
- Standards of Tubular Exchanger Manufacturers Association*, 5th edition, Tubular Exchanger Manufacturers Association, Inc., New York, N.Y., 1968.
- Perry, R.H., Chilton, C.H., and Kirkpatrick, S.D., *Chemical Engineers Handbook*, 5th edition, Sections 10 and 11, McGraw-Hill Book Co., Inc., New York, 1983.
- Peters, M.S. and Timmerhaus, K.D., *Plant Design and Economics for Chemical Engineers*, 3rd edition, Chapter 14, McGraw-Hill Book Co., Inc., New York, 1980.
- M Ganapathy, V., *Applied Heat Transfer*, PennWell Publishing Co., Tulsa, Okla., 1982.

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8. *Engineering Data Book*, 9th edition, Gas Processors Suppliers Association, Tulsa, Okla., Chapter 8, 1972.
9. Evans, Frank L., Jr., *Equipment Design Handbook for Refineries and Chemical Plants*, Volume 2, 2nd.edition, Gulf Publishing Co., Houston, Texas, 1980.

Chapter 21: Hydrotreater

The HYdroTReater module is a yield model of a unit for hydrogenation of olefinic and aromatic crude feeds and for desulfurization and denitrogenation of high-sulfur crude. The reactor is an adiabatic type with catalyst beds packed in series. Quench streams are added between beds to absorb the large amount of heat released by the exothermic reactions. The quench streams can be either the hydrogen feed or reactor products (minus hydrogen, hydrogen sulfide, and ammonia). The outlet stream from the hydrotreater is a combination of the product stream, the quench stream(s) and excess hydrogen. A second exit stream can be coded if you want to see the quench flowrate and composition.

Your COMponents command should include hydrogen, hydrogen sulfide and ammonia in addition to the components which make up your feed. You can enter as many hydrocarbon feed streams as you wish. The last stream entered **must** be the hydrogen stream. The next-to-last stream should be the hydrocarbon product flowrates on a component-by-component basis, excluding quench, excess hydrogen, ammonia, and hydrogen sulfide.

Hydrotreater Reactor Methodology

If more than one hydrocarbon feed is present (number of input streams is greater than 3), the hydrocarbon feeds are mixed. The hydrogen stream (composition and flowrates have been specified by the user) is then mixed with the hydrocarbon feed(s). If the resulting hydrogen partial pressure is too low for the reactor, the program calculates a new flowrate for the hydrogen stream; composition remains the same, total flowrate changes.

The program uses the extent of reaction and feed information (specified by the user) to determine the heat released by the reactions as well as flowrates for ammonia and hydrogen sulfide. The program makes iterative calculations around each catalyst bed, determining the required quench flowrate, the percent completion of the reactions, and the heat of reaction for each bed. The outlet stream from the hydrotreater will consist of the hydrocarbon product plus quench and excess hydrogen.

Hydrotreater Reactor Command Details

Hydrotreater: Extent of Reaction Commands

(enter **all** of the following)

SULfur **RE**acted = *fraction*

Enter the fraction of sulfur that is converted to H₂S.

NITrogen **RE**acted = *fraction*

Enter the fraction of nitrogen that is converted to NH₃.

OLEfin **RE**acted = *fraction*

Enter the fraction of olefins that is saturated/ hydrogenated.

AROmatic **RE**acted = *fraction*

Enter the fraction of aromatics that is hydrogenated.

Feed Description

SULfur **CON**tent = *fraction*

Enter the weight fraction of sulfur in the feed.

NITrogen **CON**tent = *fraction*

Enter the weight fraction of nitrogen in the feed.

OLEfin **CON**tent = *fraction*

Enter the mole fraction of olefins in the feed.

AROmatic **CON**tent = *fraction*

Enter the mole fraction of aromatics in the feed.

Hydrotreater: Quench Commands

OPTion **QUE**nch =

Enter your option for composition of the quench stream(s): (Default is 0)

0 specifies a quench composed of reactor product stream minus excess H₂, H₂S and NH₃

1 specifies hydrogen quench.

NOTE: If you specify hydrogen quench, you must also specify hydrogen stream composition and flowrates with a FLOWrate command in the GENeral section of the input file.

TEMperature of **QUE**nch (T units) =

Enter the temperature of the quench stream.

PREssure of **QUE**nch (P units) =

Enter the pressure of the quench stream.

Hydrotreater: Catalyst Bed Commands

OPTion for temperature **RIS**e per bed =

Enter your option for temperature control in each bed:

- 0** specifies a constant temperature rise for each bed.
- 1** if you are specifying the maximum number of beds along with a temperature rise for each bed.
- 2** if you want the program to calculate the number of beds required. You will have to specify a temperature rise for all beds except the last one.

OPTion for temperature **DRO**p per quench =

Enter your option for temperature control with quench.

- 0** for constant temperature drop per quench.
- 1** if you want to specify a temperature drop for each quench.

PREssure **DRO**p per bed (P units) =

Enter the pressure drop per bed (one value only).

OPTIONAL COMMAND DETAILS

Some of the Optional commands are required, depending on your entries for OPT RIS and OPT DRO.

Hydrotreater: Option for Temperature Rise per Bed Specifications

MAXimum number of beds =

Enter the maximum number of beds (10 are allowed). This command must be used when OPT RIS = 1.

number of **BED**s in reactor =

Enter a guess for the number of beds in the reactor. This command is used when OPT RIS = 2

TEMperature **RIS**e per bed (T units) =

Enter the temperature rise per bed with entries separated by commas. This command must be used when OPT RIS = 1 or 2.

CONstant temperature **RIS**e (T units) =

Enter the permissible temperature rise between beds. This command must be used when OPT RIS = 0.

Hydrotreater: Option for Temperature Drop per Quench Specifications

TEMperature **DRO**p per quench (T units) =

Enter the temperature drop per quench, with entries separated by commas. This command must be used when OPT DRO = 1.

CONstant temperature **DRO**p (T units) =

Enter the temperature drop between beds. This command must be used when OPT DRO = 0.

Hydrotreater: Print Options

PRInt =

Enter your option to control the printout information for the hydrotreater. Enter a

- 0** for combined feed information, including hydrogen, and a plot of the beds.
 - 1** for minimum printout (revised product stream and a plot of the beds).
 - 2** for feed information, a plot of each bed and *product* information between beds.
-

Hydrotreater Reactor Command Summary

Extent of Reaction

SULfur **REA**cted = *fraction*

NITrogen **REA**cted = *fraction*

OLEfin **REA**cted = *fraction*

AROmatic **REA**cted = *fraction*

Feed Description

SULfur **CON**tent = *weight fraction*

NITrogen **CON**tent = *weight fraction*

OLEfin **CON**tent = *mole fraction*

AROmatic **CON**tent = *mole fraction*

Quench Description

OPTion **QUE**nch = *0 or 1*

TEMperature of **QUE**nch (T units) =

PREssure of **QUE**nch (P units) =

Catalyst Bed Description

OPTion for temperature **RIS**e per bed = *0, 1, or 2*

OPTion for temperature **DRO**p per quench = *0 or 1*

PREssure **DRO**p per bed (P units) =

Temperature Rise per Bed Specifications

MAXimum number of beds =

number of **BED**s in reactor =

TEMperature **RIS**e per bed (T units) =

CONstant temperature **RIS**e (T units) =

Temperature Drop per Quench Specifications

CONstant temperature **DRO**p (T units) =

TEMperature **DRO**p per quench (T units) =

Print Options

PRInt = *0, 1, or 2*

Hydrotreater Reactor Step by Step

Hydrotreater Reactor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
Equipment number
Equipment name
Inlet stream
Outlet streams

HYTR

Assigned equipment flowsheet number
User choice - up to 16 characters
Unlimited in Number
One or two

Inlet stream coding specifications

- Last stream entered must be hydrogen
- Next-to-last stream entered must be the estimated hydrocarbon product.

Hydrotreater Reactor STEP 2

Enter all the required specifications at the right.

Extent of reaction specifications (enter ALL of the following).

Fraction of sulfur which is converted to H₂S
Fraction of nitrogen which is converted to NH₃
Fraction of olefins which are saturated/hydrogenated
Fraction of aromatics which are hydrogenated

SUL REA = fraction
NIT REA = fraction
OLE REA = fraction
ARO REA = fraction

Feed description specifications (enter ALL of the following)

Weight fraction of sulfur in the feed
Weight fraction of nitrogen in the feed
Mole fraction of olefins in the feed
Mole fraction of aromatics in the feed

SUL CON = fraction
NIT CON = fraction
OLE CON = fraction
ARO CON = fraction

Quench description specifications (enter ALL of the following)

Quench stream(s) composition (enter ONE of the following)

Quench composed of reactor product stream minus excess H₂, H₂S and NH₃ (default)
Hydrogen quench (hydrogen stream composition and flowrates must also be specified with a FLOWrate command)

OPT QUE = 0
OPT QUE = 1

Quench stream temperature

TEM QUE (T units) =

Quench stream pressure

PRE QUE (P units) =

Catalyst bed specifications enter ALL of the following)

Option for temperature control in each bed (enter **ONE** of the following)

Constant temperature rise for each bed
Maximum number of beds with a temperature rise for each bed
Program calculates number of beds required (a temperature rise must be specified for all beds except the last one)

OPT RIS = 0
OPT RIS = 1
OPT RIS = 2

Temperature control with quench option (enter **ONE** of the following)

Constant temperature drop per quench
Temperature drop for each quench to be specified
Pressure drop per bed (one value only)

OPT DRO = 0
OPT DRO = 1
PRE DRO (P units) =

Choose any of the optional specifications listed below, depending on the entries for OPT RIS and OPT DRO.

If OPT RIS = 0, THEN enter the following:

The temperature rise in each bed and, optionally, a guess for the number of beds

CON RIS (T units) =
BED =

If OPT RIS = 1, THEN enter the following:

Maximum number of beds (10 are allowed)

MAX =

If OPT RIS = 1, or IF OPT RIS = 2, THEN enter the following

Temperature rise per bed with entries separated by commas

TEM RIS (T units) =

If OPT DRO = 0, THEN enter the following:

Permissible temperature drop between beds

CON DRO (T units) =

If OPT DRO = 1, THEN enter the following:

Temperature drop per quench with entries separated by commas

TEM DRO (T units) =

Print option (enter ONE of the following)

Combined feed information, including hydrogen, and a plot of the beds
Minimum printout (revised product stream and a plot of the beds)
Feed information, a plot of each bed and product information between beds

PRI = 0
PRI = 1
PRI = 2

Hydrotreater Example: Crude Treating

There are several sample flowsheets in “Chapter 26: Hydrotreater Samples - c:\designii\samples\equipmnt\hytr” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 22: Line Pressure Drop

The LINE module calculates **pressure drops** due *to friction* and elevation changes (if any) in transmission lines or plant piping of specified length and diameter. The LINE module can have one or more inlet streams and has one stream out. Multiple inlet streams will be mixed together at the lowest inlet stream pressure. The LINE module can be connected to any other equipment modules, such as PUMPs, COMPRESSOR stations, HEAT EXCHANGERS and FLASH separators to simulate a complete transmission line. Simple networks and gathering systems can also be modeled as integrated flowsheets consisting of one or more LINE modules with branches, junctions and intermediate equipment. The pressure drops in plant piping can be modeled as part of the process flowsheet by using LINE modules. The resulting outlet pressure is then used in downstream calculations.

Line Pressure Drop Features

The LINE module calculates pressure drops due to friction and elevation changes (if any) in transmission lines or plant piping of specified length and diameter. The LINE module can have one or more inlet streams and has one stream out. Multiple inlet streams will be mixed together at the lowest inlet stream pressure. The LINE module can be connected to any other equipment modules, such as PUMPs, COMPRESSOR stations, HEAT EXCHANGERS and FLASH separators to simulate a complete transmission line. Simple networks and gathering systems can also be modeled as integrated flowsheets consisting of one or more LINE modules with branches, junctions and intermediate equipment. The pressure drops in plant piping can be modeled as part of the process flowsheet by using LINE modules. The resulting outlet pressure is then used in downstream calculations.

The stream(s) entering the LINE module can be gas, liquid, or two-phase. Phase change, such as flashing condensate or retrograde condensation in the LINE module, is detected and reported if it occurs. Pressure drop and flow regime are predicted along the line by repeating the calculations at each node or point along the LINE. Calculations can be isothermal, adiabatic, or based on heat transfer to the surroundings and several calculation methods can be selected by the user. The method options currently available are primarily applicable to hydrocarbon and hydrocarbon-water systems.

Several line sections of different lengths and elevations can be modeled in a single LINE module. Results are tabulated for each of the node points specified along the line.

Unless the Beggs and Brill calculation technique is specified, the Baker flow regime map is given for each two-phase horizontal LINE module to show the proximity to flow regime boundaries. Beggs and Brill employs somewhat different flow regime labels.

Sizing calculations or back pressure calculations can be performed using a CONTROLLER module to vary inlet conditions to the LINE module (varying specifications for COMPRESSOR, DIVIDER, STREAM manipulator) until the required outlet conditions are met. You can also use the new PRESSURE OUT command and Inline FORTTRAN (CALUPS PRG) to reset the outlet pressure for a PUMP COMPRESSOR, or VALVE. Add a MAX = X and RECYCLE SEQ = command in the GENERAL section to force recalculation of the upstream equipment and LINE module.

Diameter case studies are also allowed in the same LINE module. Results for all cases will be reported in the LINE module output. The outlet pressure reported in the stream summary will be the outlet pressure calculated for the last case.

Pressure and elevation profiles along the line can be plotted according to user specifications. Points on the curve correspond to the node points calculated in the LINE module. Points from several LINE modules in the same run can be included in a single profile plot for a typical transmission line.

The main capabilities of the LINE module can be summarized as follows:

- Two phase, gas or liquid line pressure drop
- Integrated models, including intermediate equipment, branches and junctions.
- Complete flowsheet flexibility
- User choice of methods for pressure drop
- Back pressure calculations
- Diameter case studies
- Phase determination and property calculation at each node Two phase flow regime map
- Plots of key variables against length for one or more LINE modules
- Liquid holdup and slug characteristics for two phase lines in slug or plug flow regimes

Calculation Method

The calculation methods used are primarily applicable to hydrocarbon systems in fairly small diameter lines, and results will vary with the density and viscosity correlations you choose for the simulation. Also, results of two phase and non-isothermal calculations will vary with the K-value and enthalpy correlations, respectively.

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.

Physical properties of the fluid are obtained automatically from DESIGN II inlet stream information and do not have to be entered. Subsequent isothermal flashes (default), adiabatic flashes or heat exchange calculations are performed at each of

Chapter 22

the LINE nodes and phase properties are calculated. The thermodynamic options you choose in the GENeral section will be used to generate Kvalues and enthalpies. For heat and material balance calculations the Kvalues and enthalpies are the most important properties. For calculating pressure drops in lines, other physical properties, particularly density and viscosity, are also important. Some guidelines for density choices follow:

COPED

Used for natural gas mixtures up to about 400 F, if the mixture does not contain large amounts of CO₂ or H₂S.

BWRSD

Used for most hydrocarbon and inorganic gases at high pressures.

STDD

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 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. It is not suitable for polar mixtures.

The Dean and Stiehl technique was developed for estimating vapor viscosities. It is generally poor for estimating liquid viscosities and should not be used for LINE calculations.

The API technique is the default viscosity option when your input includes CRUde, REFIne, or PETroleum STReam commands. If the feed contains significant amounts of light components (methane through pentanes, CO₂, H₂S, and N₂), 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

MODified API is an updated version of the API *Technical Data Book* methods for calculating vapor and liquid viscosities for heavy hydrocarbon streams (4th ed.).

If the stream contains a large amount of water, you should consider using one of the methods available in LINE module for handling oil-water emulsions.

The pressure drop in a line section is considered to be due to the effects of friction and elevation. Any pressure drop due to acceleration is ignored by default. If pressure drop due to acceleration is significant for a specific application, you may specify that it should be considered.

Sonic velocity in the gas phase is estimated using the generalized correlation of T. K. Sherwood (Reference 8). Each line node is checked to make sure that the flow is subsonic, and sonic velocity is reported at the inlet/outlet conditions. Stream entry, exit and line node velocities are also displayed in the pressure drop table.

Line Pressure Drop Command Details

Several commands define the length, size, direction and other characteristics of the LINE to be calculated. A diameter (either DIA or INS) and the LENgth of the LINE must be specified. A chart of the available nominal DIAMeters and PIPE WALl thickness codes is shown in the *Line: Nominal Pipe Diameter Table*

Multiple values can be entered on the nominal DIAMeter or INSide diameter commands for case studies. DESIGN II will then calculate the pressure drop for each pipe diameter, using the values you have given for the other commands. When using the case study option, entering the diameters in smallest to largest order is advisable, as the calculated outlet pressure of the last case is the value which is passed to the next module. For a given flow, the pressure drop will be least for the largest diameter pipe.

nominal **DIAMeter** (L units) =

Enter the nominal diameter for the LINE.

or

INSide diameter (L units) =

Enter the specified inside diameter of the pipe. The default value is the inside pipe diameter corresponding to the pipe wall thickness code. Use this command if the nominal diameter exceeds 48 inches.

Multiple values can also be entered for the LENgth command, but these values indicate the length of each node in the LINE, not the length of the LINE for the first diameter. Sections of a line are determined mainly by elevation or direction changes, but long line sections with large pressure drops should also be broken into several length sections to obtain more accurate results. You should break the LINE in increments so that the pressure drop for a node does not exceed ten percent (10%) of the inlet pressure to that node. Alternatively, use the optional SEGment LENgth or SEGment ELEvation commands to break the LINE into a reasonable length between nodes.

LENgth of line sections (L units) =

Enter the length of each section of same diameter line from node to node. Line nodes are defined by the line sections entered with the LENgth command. The number of nodes is the number of values entered plus 1.

Line Pressure Drop Optional Command Details

Line: Equivalent Length Command

EQUIvalent length (L units) =

Enter the equivalent length of bends and fittings for each section of same diameter line from node to node. These values will be added to the actual length for calculations. Default is zero.

Line: Equivalent Length Table Table 1

EQUIPMENT NUMBER: 2 INLET STREAM(S): 2
 NAME: SEC 1 OUTLET STREAM(S): 3
 K-VALUES: SOAVE ENTHALPY: SOAVE VAP DEN: STD LIQ DEN: STD

NO. OF SEGMENT (USER SPECIFIED) = 10
 TOTAL LENGTH FT = 52800.
 OVERALL ELEVATION FT = 16.000
 TOTAL EQU. LENGTH FT = 550.00
 SEGMENT LENGTH FT = 5280.0
 TYPE OF CALCULATION = ADIABATIC

CASE STUDY (DIAMETER) = 1

NOMINAL DIAMETER FT	FRICTIONAL DELTA P PSI	ELEVATION DELTA P PSI	ACCELERATION DELTA P PSI	TOTAL PSI
1.0000	359.38	0.57025	0.00000	359.95

=====
 The Now Calling results
 =====

NOW CALLING EQUIPMENT 2 + LIN = SEC 1 15:30:24
 KVALUES: SOAVE ENTHALPY: SOAVE VAP DEN: STD LIQ DEN: STD

LIN 2 = SEC
 RESULTS OF LINE 2 - GAS FLOW
 INLET STREAM(S) 2
 OUTLET STREAM(S) 3
 LINE CHARACTERISTICS: HORIZONTAL

ADIABATIC
 ELEVATIONS ARE REPORTED RELATIVE TO INLET NODE.

VAPOR FLOWRATE SCF/HR	3.8738E+06	LIQUID FLOWRATE GAL/HR	0.0000
PIPE ROUGHNESS FT	1.5000E-04	PIPE EFFICIENCY FACTOR	1.000
INTERNAL DIAMETER INCHES	12.000	OUTSIDE DIAMETER INCHES	12.750
NOMINAL DIAMETER INCHES	12.000	PIPE WALL THICKNESS CODE	STD

METHODS FOR:	FRICTION DELTA P	FRICTION FACTOR	ELEVATION DELTA P
	DARCY	MOODY	PHASE DENSITY

PRESSURE DROPS ARE REPORTED AS FROM THE PREVIOUS NODE TO THE CURRENT NODE.

LINE NODE	LENGTH FT	ELEV. FT	TEMP. DEG F	DELP-FRIC PSI	DELP-ELEV PSI	PRESS. PSIA	VELOC. FT/SEC	LIQUID FLOW HOLDUP	REGIME
--------------	--------------	-------------	----------------	------------------	------------------	----------------	------------------	--------------------------	--------

Chapter 22

0	0.0	0.0	150.6			1000.00	16.8	0.0000	TURBULENT
1	5280.0	5.0	148.5	25.65	0.21	974.14	17.2	0.0000	
TURBULENT									
2	10560.0	3.0	146.3	27.21	-.81E-01	947.01	17.7	0.0000	
TURBULENT									
3	15840.0	6.0	143.9	28.40	0.12	918.49	18.3	0.0000	
TURBULENT									
4	21120.0	7.0	141.5	28.98	0.38E-01	889.48	19.0	0.0000	
TURBULENT									
5	26400.0	8.0	138.8	30.38	0.37E-01	859.06	19.7	0.0000	
TURBULENT									
6	31680.0	9.0	135.3	39.09	0.36E-01	819.94	20.7	0.0000	
TURBULENT									
7	36960.0	10.0	131.6	40.10	0.34E-01	779.80	21.8	0.0000	
TURBULENT									
8	42240.0	12.0	127.5	43.39	0.64E-01	736.35	23.2	0.0000	
TURBULENT									
9	47520.0	14.0	123.0	46.62	0.60E-01	689.67	24.9	0.0000	
TURBULENT									
10	52800.0	16.0	118.0	49.56	0.56E-01	640.05	27.0	0.0000	
TURBULENT									

REYNOLDS NUMBER TABLE

LINE NODE	LIQUID REYNOLDS NUMBER	LIQUID TRANSITION REYNOLDS #	VAPOR REYNOLDS NUMBER	VAPOR TRANSITION REYNOLDS #	FRICTION FACTOR	FLOW REGIME
0	0.0000000	0.0000000	9791375.	612337.2	0.1309859E-01	
TURBULENT						
1	0.0000000	0.0000000	9906203.	612337.2	0.1309702E-01	
TURBULENT						
2	0.0000000	0.0000000	0.1002866E+08	612337.2	0.1309538E-01	
TURBULENT						
3	0.0000000	0.0000000	0.1015956E+08	612337.2	0.1309367E-01	
TURBULENT						
4	0.0000000	0.0000000	0.1029510E+08	612337.2	0.1309195E-01	
TURBULENT						
5	0.0000000	0.0000000	0.1043973E+08	612337.2	0.1309015E-01	
TURBULENT						
6	0.0000000	0.0000000	0.1062971E+08	612337.2	0.1308787E-01	
TURBULENT						
7	0.0000000	0.0000000	0.1082924E+08	612337.2	0.1308556E-01	
TURBULENT						
8	0.0000000	0.0000000	0.1105066E+08	612337.2	0.1308309E-01	
TURBULENT						
9	0.0000000	0.0000000	0.1129491E+08	612337.2	0.1308048E-01	
TURBULENT						
10	0.0000000	0.0000000	0.1156177E+08	612337.2	0.1307775E-01	
TURBULENT						

NOTE: Transition reynolds number is not calculated for two phase flow. (szlseg)

LIN 2 = SEC

PHASE AND DENSITY TABLE

NODE	VAPOR FRACTION (MOLAR)	VAPOR FRACTION (VOLUME)	VAPOR DENSITY LB/FT3	LIQUID DENSITY LB/FT3	COMBINED DENSITY LB/FT3	LINE PACK FT3	FROUDE NUMBER
0	1.00000	1.00000	5.9998	0.00000	5.9998	0.00000	
8.7437							
1	1.00000	1.00000	5.8393	0.00000	5.8393	3.32061E+05	
9.2309							
2	1.00000	1.00000	5.6699	0.00000	5.6699	3.22812E+05	
9.7908							
3	1.00000	1.00000	5.4913	0.00000	5.4913	3.13057E+05	
10.438							

Line Pressure Drop

4	1.00000	1.00000	5.3088	0.00000	5.3088	3.02932E+05
11.168						
5	1.00000	1.00000	5.1170	0.00000	5.1170	2.92440E+05
12.021						
6	1.00000	1.00000	4.8696	0.00000	4.8696	2.80157E+05
13.273						
7	1.00000	1.00000	4.6153	0.00000	4.6153	2.66092E+05
14.776						
8	1.00000	1.00000	4.3399	0.00000	4.3399	2.51254E+05
16.711						
9	1.00000	1.00000	4.0443	0.00000	4.0443	2.35257E+05
19.243						
10	1.00000	1.00000	3.7310	0.00000	3.7310	2.18198E+05
22.610						

NOTE: The line pack value listed for each node is the average
 NOTE: line pack for the previous node and current node (szlseg)

ESTIMATED SONIC VELOCITY IN GAS PHASE
 = 940.8 FT/SEC AT INLET CONDITIONS.
 = 934.0 FT/SEC AT OUTLET CONDITIONS.

EQUIVALENT LENGTH TABLES FOR PIPING, VALVES AND FITTINGS

LINE	EQUIV.	ELL 90	ELL 90	ELL 90	ELL 45	ELL 45	ELL180	ELL180	TEE
NODE	LENGTH	R/D=1.0	R/D=1.5	MITERD	R/D=1.0	R/D=1.5	R/D=1.0	R/D=1.5	BRANCH
	FT	FT	FT	FT	FT	FT	FT	FT	FT
1	10.00	30.00	160.00	120.00	320.00	10.00	750.00	100.00	60.00
2	20.00	60.00	144.00	240.00	288.00	20.00	600.00	200.00	120.00
3	30.00	90.00	128.00	360.00	256.00	30.00	450.00	300.00	180.00
4	40.00	120.00	112.00	480.00	224.00	40.00	300.00	100.00	60.00
5	50.00	150.00	96.00	600.00	192.00	50.00	150.00	200.00	120.00
6	60.00	180.00	80.00	720.00	160.00	10.00	750.00	300.00	180.00
7	70.00	210.00	64.00	840.00	128.00	20.00	600.00	100.00	60.00
8	80.00	240.00	48.00	960.00	96.00	30.00	450.00	200.00	120.00
9	90.00	270.00	32.00	1080.00	64.00	40.00	300.00	300.00	180.00
10	100.00	300.00	16.00	1200.00	32.00	50.00	150.00	100.00	60.00

L/D
 ratio 1.00 30.00 16.00 60.00 16.00 10.00 150.00 100.00 60.00

LINE	GATE	GLOBE	ANGLE	CHE VAL	CHE VAL	
NODE	VALVE	VALVE	VALVE	SWING	LIFT	TOTAL
	FT	FT	FT	FT	FT	FT
1	8.00	1700.00	1500.00	100.00	600.00	5468.00
2	16.00	1360.00	1350.00	200.00	1200.00	5818.00
3	24.00	1020.00	1200.00	100.00	1800.00	5968.00
4	32.00	680.00	1050.00	200.00	2400.00	5838.00
5	40.00	340.00	900.00	100.00	3000.00	5988.00
6	8.00	1700.00	750.00	200.00	3600.00	8698.00
7	16.00	1360.00	600.00	100.00	4200.00	8368.00
8	24.00	1020.00	450.00	200.00	4800.00	8718.00
9	32.00	680.00	300.00	100.00	5400.00	8868.00
10	40.00	340.00	150.00	200.00	6000.00	8738.00

L/D
 ratio 8.00 340.00 150.00 100.00 600.00

Line: Elevation Change Command

If this command is used, it should have the same number of values entered as the LENgth command. A negative value indicates a decrease in elevation and a positive value indicates an increase. An inclined horizontal line can be modeled by entering elevation values for each section of line.

ELEvation (L units) =

Enter the elevation for each line section relative to the previous node. The default value is zero if no ELEvation command is entered for a HORizontal line. For a vertical (UP or DOWN) line the default is the line length.

Line: Segment Commands

These two commands allow the distance between nodes specified via the LENgth command to be subdivided into any number of segments based on either length or elevation. If either or both of these commands are entered, the LINE module will use a length equal to the shortest of the following three: specified node length, the length set by the SEG LEN command, or the length set by the SEG ELE command.

SEGment LENgth =

Enter the maximum segment length per node

SEGment ELEvation =

Enter the maximum segment elevation per node

Line: Wall Thickness Command

The default value for the inside diameter will be the value which corresponds to the default pipe wall thickness (STD) for the nominal DIAMeter you have specified. (See *Line: Nominal Pipe Diameter Table*) Specifying both the inside diameter and the PIPE WALI thickness is not recommended. Up to 14 inside diameters are available for a given nominal DIAMeter while a maximum of 3 PIPE WALI thickness codes (STD, XS, XXS) are available.

PIPE WALI thickness 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.

or

PIPE wall THickness (L units) =

Enter the desired pipe wall thickness. This option is normally used with the INS DIA command, while PIPE WALI code is used with the nominal DIAMeter specification.

Line: Nominal Pipe Diameter Table
Table 2

Nominal Pipe Diameter (Inches)	Pipe Wall Code	Wall Thickness (Inches)	Inside Diameter (Inches)
1	STD	.133	1.049
	XS	.179	.957
	XXS	.358	.599
1.5	STD	.145	1.610
	XS	.200	1.500
	XXS	.400	1.100
2	STD	.154	2.067
	XS	.218	1.939
	XXS	.436	1.503
2.5	STD	.203	2.469
	XS	.276	2.323
	XXS	.552	1.771
3	STD	.216	3.068
	XS	.300	2.900
	XXS	.600	2.300
3.5	STD	.226	3.548
	XS	.318	3.364
4	STD	.237	4.026
	XS	.337	3.826
	XXS	.674	3.152
5	STD	.258	5.047
	XS	.375	4.813
	XXS	.750	4.063
6	STD	.280	6.065
	XS	.432	5.761
	XXS	.864	4.897

Line Pressure Drop

8	STD	.322	7.981
	XS	.500	7.625
	XXS	.875	6.875
10	STD	.365	10.020
	XS	.500	9.750
	XXS	1.000	8.750
12	STD	.375	12.000
	XS	.500	11.750
	XXS	1.000	10.750
14	STD	.375	13.250
	XS	.500	13.000
16	STD	.375	15.250
	XS	.500	15.000
18	STD	.375	17.250
	XS	.500	17.000
20	STD	.375	19.250
	XS	.500	19.000
24	STD	.375	23.250
	XS	.500	23.000
26	STD	.375	25.250
	XS	.375	25.000
28	STD	.375	27.250
	XS	.500	27.000
30	STD	.375	29.250
	XS	.500	29.000
32	STD	.375	31.250
	XS	.500	31.000
34	STD	.375	33.250
	XS	.500	33.000
36	STD	.375	35.250
	XS	.500	35.000

Line: Flow Direction Commands

Only one direction of flow is allowed per LINE module. If the line changes flow direction, different LINE modules should be used for each change. Choices are HORIZONTAL, UP or DOWN. Use of the ELEVATION command with the HORIZONTAL direction would indicate an inclined or sloping LINE. The default flow direction is HORIZONTAL and the default elevation for a horizontal line is zero. For vertical lines (UP or DOWN), the default elevation is assumed to be the LENGTH of the LINE (for each node). Negative values indicate a drop in elevation; positive values indicate a rise in elevation.

HORIZONTAL

This is the default line direction. It includes inclined horizontal.

UP

Vertical upwards flow, including inclined upwards flow.

DOWN

Vertical downwards flow, including inclined downwards flow.

Line: Pipe Transport Efficiency Commands

Three transport efficiency values are optional in the LINE module: roughness, drag factor, and pipeline efficiency.

ROUGHNESS (L units) =

Enter the absolute roughness of the pipe (or effective roughness if using the AGA friction pressure drop equation).

Default is 0.00015 feet. See *Line: Typical Absolute Surface Roughness Values Table*.

If you specify METHOD for FRICTIONAL pressure drop = AGA, specify a more conservative value for ROUGHNESS. The

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roughness term in the AGA equation is the effective roughness, which may be higher due to welds, fittings, deposits, dirty gas, and years of service. Typical values for effective surface roughness are given in *Line: Typical Effective Roughness Values for Use in the AGA Equation*.

Line: Typical Absolute Surface Roughness Values Table
Table 3

Pipe Type	Absolute Roughness(feet)
Drawn Tubing	.000005
Commercial Steel	.00015
Asphalted Cast Iron	.0004
Galvanized Iron	.0005
Cast Iron	.00085
Concrete	.001-.01
Riveted Steel	.003-.03

Also, see *Line: Typical Effective Roughness Values for Use in the AGA Equation*.

Line: Typical Effective Roughness Values for Use in the AGA Equation
Table 4

Pipe Type and Condition	Estimated Roughness (inches)
Bare Steel Pipe - New	.000500 - .000750
Bare Steel Pipe: Exposure Time to Typical Climatic Conditions:	
6 months	.001000 - .001250
12 months	.001500
24 months	.001750
Plastic-Lined Pipe	.000200 - .000300
Sandblasted Pipe	.000200 - .000300
Pig-Burnished Pipe	.000300 - .000500

In addition to modifying the ROUghness value when you are specifying MET FRI = AGA, you can enter a value for the DRAg factor. The drag factor is used to determine the transition Reynolds number and to predict the AGA friction factor when flow is partially turbulent. A value in the range of 0.9 to 0.985 is appropriate.

DRAg factor

Enter the appropriate fraction for use in the AGA equation. The default is 1.0. (See Figure 1).

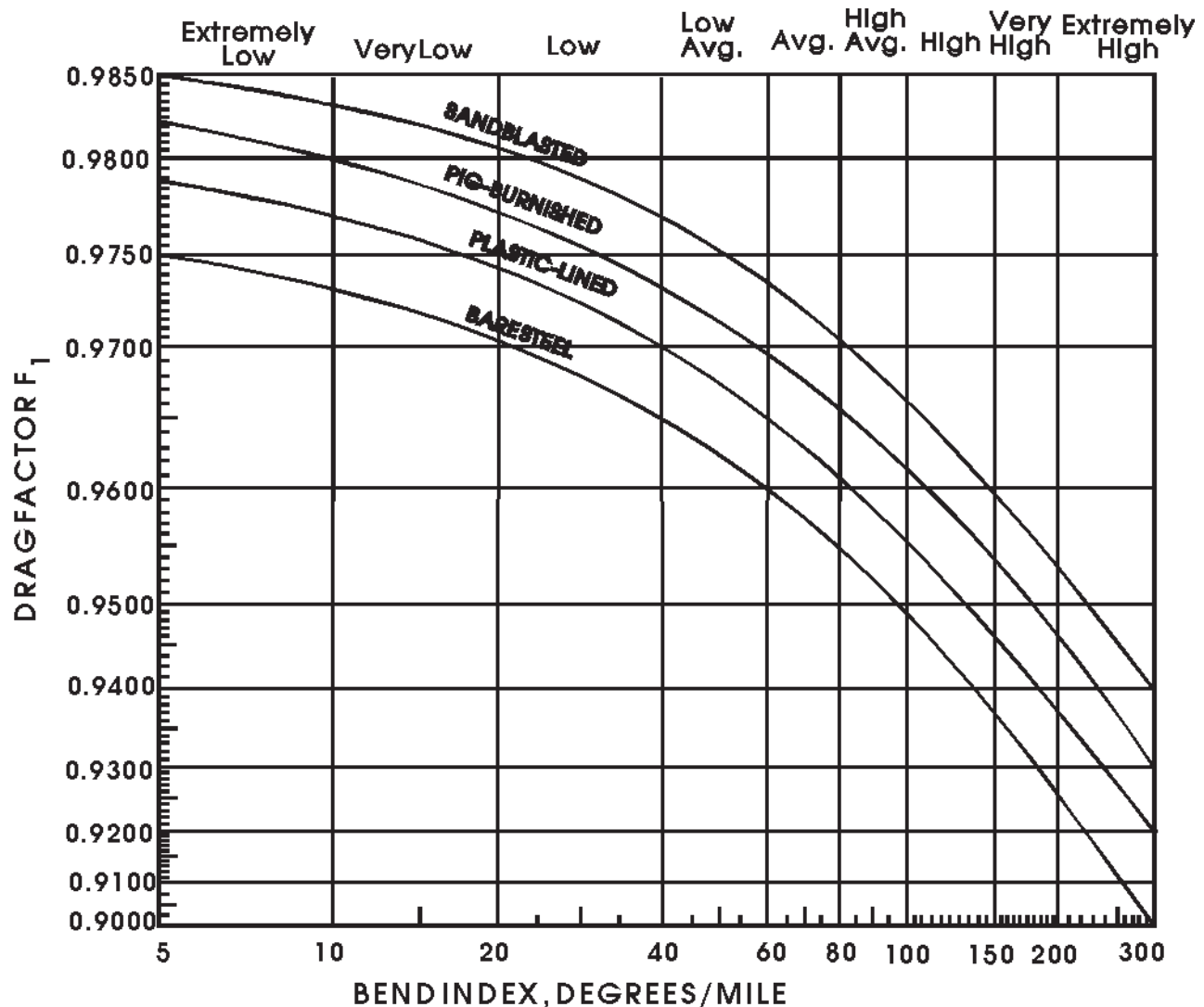


Figure 1. Drag Factor as a Function of Pipe Type and Bend Index (For typical transmission lines onstructed of 40 - foot pipe joints welded in the field with a valve setting approximately every 10 miles)

A pipeline (flow) Efficiency can be entered for use in calculation of frictional pressure drop with the PANhandle A or MODified Panhandle equations. This EFFiciency will also be used in the WEYmouth equation. Some typical values for EFFiciency are shown in *Line: Typical Pipeline Efficiency Values Table*.

pipeline **EFFiciency** =

Enter the fractional pipeline efficiency . Default is 1.

Line: Typical Pipeline Efficiency Values Table
Table 5

Pipeline Conditions	Efficiency
New pipe without any bends, elbows, valves, changes of diameter or elevation	1.00
Very good operating conditions	0.95
Clean "pipeline quality" gas in new pipe	0.94
Average operating conditions	0.92
Rich gas, old pipe, less ideal situations	0.88
Unusually unfavorable operating conditions	0.85
Wet gas line - Use a value somewhat less than	0.85

Line: Phase Commands

Normally, the phase of the material in the LINE is determined by the program for each node in the calculation. For cases where the stream is close to single phase conditions (vapor mole fraction 0.01 or, you may want the calculations performed as if the system were single phase. To force the phase of the calculation, use the SET PHase = command. The options are VAPor or LIQuid. This command is normally not needed.

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SET PHase of calculation =

Enter either **LIQ**uid or **VAP**or to set the phase of calculations in each line section. The predicted vapor fraction must be under 0.1 for LIQ or over 0.9 for VAP, otherwise this command is ignored. The default option is the predicted phase at each node.

Line: Pipeline Heat Transfer to the Surroundings

Temperature Calculation Method (Select ONE Of The Following options)

ISO

Isothermal calculations (no heat transfer; no temperature change; default)

ADI

Adiabatic calculations (no heat transfer; temperature change due to pressure drop/rise only). Note that a temperature change can be caused by a significant change in elevation.

TEMperature of SURroundings (T units) =

Enter a value for each node in the Line (same number of values as you specified in the LENgth command).

You must also specify heat transfer coefficient values or provide information so that the heat transfer coefficients can be calculated. See section *Line: Calculate U*

U (U units) =

Enter a value for the heat transfer coefficient for each node in the line. These values will include film resistance, pipewall resistance, insulation resistance (if any), and resistance due to surroundings.

Allowable units are: BTU/HR/FT²/f (default) Kcal/HR/m²/c KJ/SEC/m²/K

Line: Calculate U

DESIGN II estimates the overall heat transfer coefficient, U, if it is not specified. Insulation thickness of each layer may be specified. There is no limit on the number of insulation layers allowed. You should also specify the nature of the surroundings and its thermal conductivity in order for DESIGN II to compute the resistance to heat transfer due to surroundings. If you choose not to specify values, DESIGN II provides default thermal conductivity values for soil, water and air.

The overall heat transfer coefficient, U, is defined as: $U = 1/R$

where R is the total resistance to heat transfer. R is the sum of the following components;

- a) Resistance due to the inside pipe film.
- b) Resistance due to the pipe wall.
- c) Resistance due to insulation layers.
- d) Resistance due to surroundings.

Pipe Details

PIPE MATerial = 'material

Enter the keyword corresponding to the pipe material. Default is **CAR**bon steel.

Material Keyword in bold	Average Thermal Conductivity (BTU/FT/HR/F)
ADMiralty brass	70.00
ALUminum	109.00
ALLoy 825	8.10
CARbon steel (default)	26.00
CARbon MOLy steel	25.00
COPper	225.00
COPper nickel 90/10	41.00
COPper nickel 70/30	17.00
MONel	15.00
NICKel 200	35.00
RED brass	92.00
STAINless steel 304	10.00
STAINless 214	21.00
TITanium	11.50
PVC	0.10
GLAss	0.6667

Pipe Thickness

Choose one of the two options:

PIPE WALl Thickness = STD, XS, or XXS

Specify pipe wall thickness code. **STD** is default (Use only with DIA specification)

or

PIPe THickness (L units) =

Specify pipe wall thickness giving measured width. (Use with either DIA or INS options)

Optional Pipe Insulation

Define insulation thickness:

INSulation THickness (L units) n =

insulation thickness of the nth layer.

INSulation CONductivity (k units) n =

thermal conductivity of the nth layer.

Where "n" is the layer number of the insulation, with 1 as the innermost layer.

NOTE: number of values entered for INSulation THickness or CONductivity commands must equal number of segments entered in the LINE module.

Surroundings Details

Surroundings may be oil, water or soil. For pipe which is submerged in water or exposed to air, you must provide information on the velocity of the surroundings. For pipe buried under soil or water, you must provide the depth of burial.

VELocity of SURroundings (L units/T units) =

Enter a value for each node in the line. Default is 0.0. Remember that default limits are feet, default t unit is HR.

or

PIPe DEPth (L units)

Enter a value for each node in the line for the depth of the pipe buried under soil or water.

Depth is measured from the surface of the soil or water to the top of the pipe. If insulation is added to the pipe, then the depth is measured to the top of the insulation.

You must also provide values for the thermal conductivity of the surroundings, either by providing explicit values for air, soil or water or by choosing to use program defaults (1 value for air or water, 6 values for soil, depending on soil type and moisture content.)

Thermal Conductivity of Surroundings

To specify the thermal conductivity of the surroundings, enter the following commands:

SURrounding SOIL CONductivity (k units) =

Enter values for thermal conductivity for soil for each node.

SURrounding WATER CONductivity (k units) =

Enter values for thermal conductivity for water for each node.

SURrounding AIR CONductivity (k units) =

Enter values for thermal conductivity for air for each node.

Only the following units are allowed for thermal conductivity input units (k units):

BTU/HR/FT/F British (default)

KJ/S/M/K SI

KCAL/HR/M/C Metric

If you wish to use default values for thermal conductivity, then one or more of the following commands must be added to the LINE module:

SUR SOIL = option

Choose default thermal conductivity value for soil.

where 'option' is one of the following keywords:

SANd 1 (sandy dry k = 0.1625 BTU/HR/FT/F)

SANd 2 (sandy moist k = 0.275)

SANd 3 (sandy soaked k = 0.6)

CLAY 1 (clay dry k = 0.125)

CLAY 2 (clay moist k = 0.225)

CLAY 3 (clay soaked k = 0.375)

If you do not want to enter specific values for air or water thermal conductivities, use a command for the default thermal conductivity.

SURrounding WATER

Choose default thermal conductivity value for water. (k=0.3517)

SURrounding AIR

Choose default thermal conductivity value for air. (k=0.015)

Line: Calculation Method Option Commands

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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).

All of the gas methods can be used to model 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. Lines which are almost all vapor (at vapor fraction 0.99999 and above), and lines which are almost all liquid (at vapor fraction 0.001 and below) are automatically calculated as single phase.

METhod for **FRI**ction pressure drop =

Enter one of the options for calculation of pressure drop due to friction. The default method is dependent on phase and direction of flow. (choose one of the following)

DARcy Weisbach

Default equation for single phase flow, suitable for all flow regimes where calculated pressure drop is under 10% of the inlet pressure (Reference 9). It is least accurate in the transition zone from partially to fully turbulent flow.

LOCKhart-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 24) is used in the wave flow regime.

ORKiszewski

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: Griffith (Reference 11) for bubble flow, Orkiszewski for slug flow friction gradient, and Duns and Ros (Reference 13) for transition and annular mist flow, and flow regime determination. The author claims approximately 10% precision in predicting pressure drops in flowing and gas lift production wells.

American Gas Association

Equation for calculating pressure drop (and also elevation pressure drop) calculated by the general flow equation. This is for both fully and partially turbulent gas flow. The AGA elevation pressure drop method is automatically used with it unless a different method for elevation delta P is specified. DRAG factor, which is normally in the range 0.9 to 0.985, should be specified whenever MET FRI = AGA is used. (Reference 16)

WEYmouth

Equation for frictional pressure drop in gas lines developed by Weymouth (Reference 7). This is the GPSA version (Reference 9) which includes the effects of compressibility factor (Z) and gas gravity. The equation is suitable for fully turbulent flow in short pipelines and gathering systems giving somewhat conservative results.

PANhandle A

Equation for frictional pressure drop in gas lines, mainly applicable to long, large diameter (6 to 24 inch) transmission lines. It is an empirical equation mainly appropriate for partially turbulent flow with Reynolds numbers in the range of 5E6 to 14E6. The original equation assumes an average temperature of 60 F 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 be specified for this equation. (Reference 9)

MODified 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 long, large diameter lines in transmission and gas delivery. It includes the effect of gas compressibility and is recommended for fully turbulent flow. Pipeline EFFiciency should be specified for this equation.

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.

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)

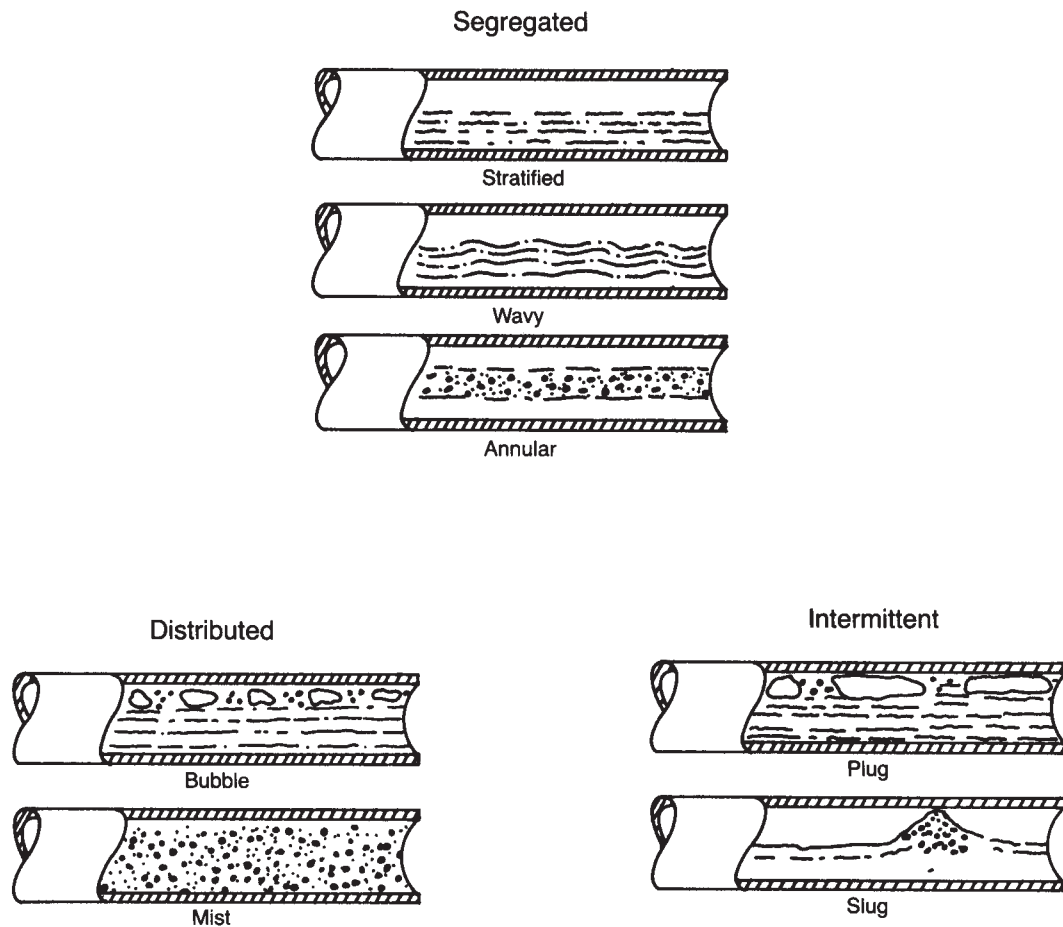


Figure 2. Beggs and Brill flow regimes

MUKherjee Brill

Mukherjee-Brill is used for two phase flow in horizontal, inclined, or vertical pipes. (Reference 23).

HAGedorn Brown

Hagedorn Brown is used for two phase flow in vertical pipes. (Reference 24)

DUNs 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)

OLIemans

Oliemans is used for two phase flow in horizontal pipes. (Reference 26)

Line: Default Methods of Calculation Table
Table 6

Phase/Direction of flow	Method	Application
Gas (includes cases which are almost all vapor)	Darcy-Weisbach Phase density	pressure drop due to friction. pressure drop due to elevation change
Liquid (includes cases which are almost all liquid)	Darcy-Weisbach Phase density	pressure drop due to friction. pressure drop due to elevation change
Two phase/Horizontal	Lockhart-Martinelli Baker Hughmark Phase density	pressure drop due to friction flow regime liquid holdup pressure drop due to elevation change
Two phase/Vertical	Orkiszewski	pressure drop due to friction

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.

JAI

Explicit friction factor comparable to the Colebrook equation in the Reynolds number range of 5000 to 10⁸ with relative roughness between 10⁻⁶ and 10⁻². (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.

Specify Secondary Pressure Drop Method and Secondary Friction Factor Method.

The LINE module allows the specification of two friction pressure drop and friction factor methods. For example, you can specify one method to be applied in the single phase region and an alternate method to be applied in the two phase region. DESIGN II will evaluate the phase at each node of the LINE module and will use the appropriate specified method.

If neither method specified is suitable for the point of evaluation, then the applicable default method will be used. If the phase shifts back to the original state, then the method will be reset to your first choice.

MET FRI =

Specify first frictional pressure drop method

MET FRI ALT =

Specify second frictional pressure drop method

MET FRA =

Specify first frictional factor method

MET FRA ALT =

Specify second frictional factor method

NOTE: The available methods are the same as listed above under Pressure drop due to Friction and Friction Factor.

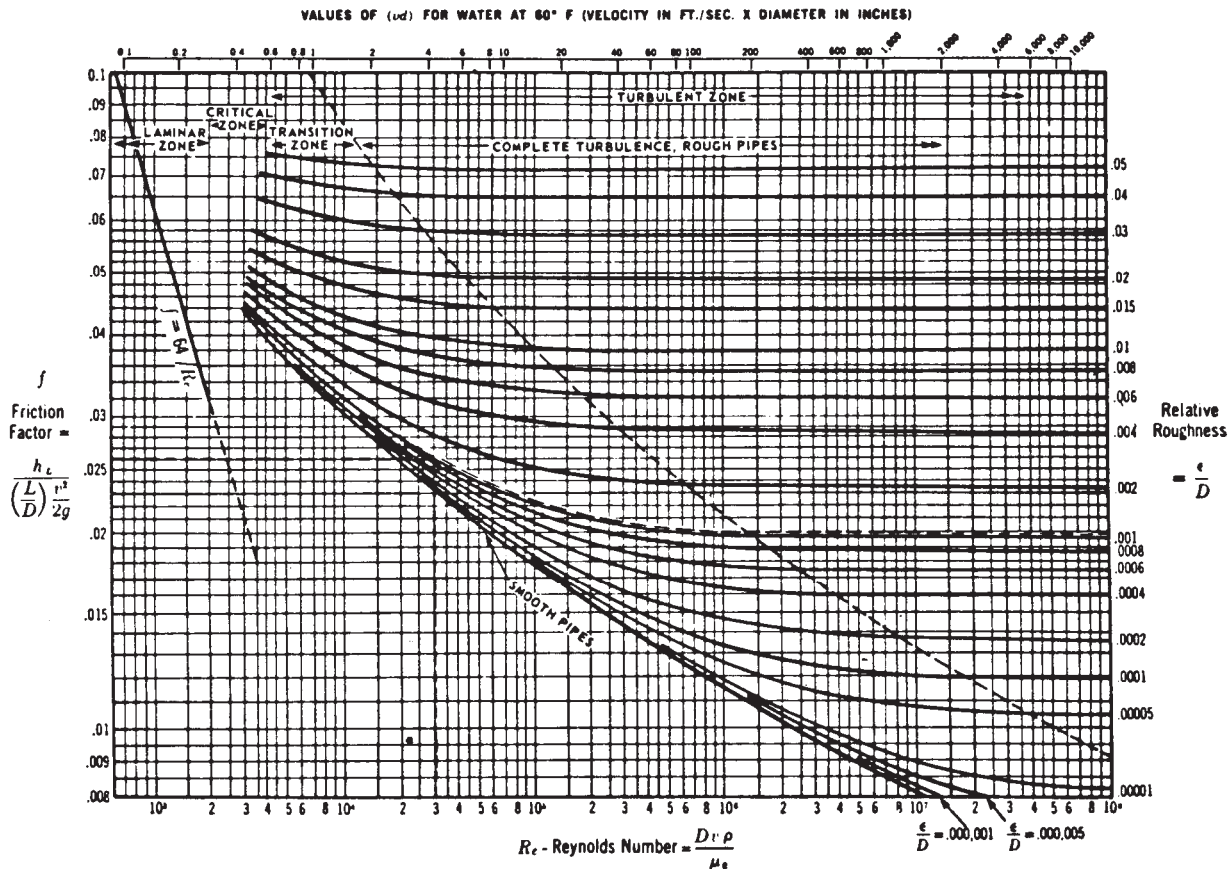


Figure 2. Moody Friction Factor Chart

Line: Pressure Drop due to Elevation Change

Several techniques are available for estimating the pressure drop (or rise) due to elevation.

METHOD for ELEVATION =

Enter one of the options for calculation of the pressure drop due to elevation. The default is PHASE density. (choose one of the following)

PHASE density

This is the default method for both single and two phase flow. In the case of two phase flow, an average phase density is used which is based on the liquid holdup volume fraction. For single phase flow, the liquid or vapor density is used. This method is recommended for all process plant line sizing and for most other situations.

FLANIGAN

This method 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 for 4 to 10 inch diameter pipe with gas velocities up to 12 feet per second and liquid to gas ratios of 20 to 1200 barrels per million standard cubic feet of gas (BBL/MMSCF). Outside the range of this data, the validity of the method is questionable.

AGA

Method for gas transmission lines when MET FRI = AGA has been specified. This incorporates elevation effects into the AGA equation. (Reference 16)

ORKISZEWSKI

Method for vertical, upwards flow in the slug flow regime. This method (Reference 4) uses the average density term of Griffith and Wallis (Reference 12) which predicts higher densities and consequently higher elevation pressure drops than the PHASE density method.

Line: Liquid Holdup Calculation Method Commands

METHOD for HOLDUP =

Enter one of the options for calculation of liquid holdup. (choose one of the following)

HUGHMARK

Default liquid holdup method. (Reference 3)

DUKLER

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Liquid holdup calculation method corresponding to the Dukler equation for frictional pressure drop. This is used automatically if MET FRI = DUK is entered. The DUKler correlation is the constant slip (Case II) method. (Reference 17)

EATon

Liquid holdup calculation method corresponding to the Eaton equation. (Reference 21)

HUGHmark and PRESSburg

Liquid holdup calculation method corresponding to the Hughmark and Pressburg equation. (Reference 22)

MUKherjee Brill

Liquid holdup method. For two phase flow in horizontal, inclined, or vertical pipes. (Reference 23.)

DUNs Ross

Liquid holdup method. For two phase flow in vertical pipes.

LOCKhart Martinelli

Liquid holdup method. For two phase flow in horizontal pipes.

Flow Regime methods (Determined by choice of Frictional pressure drop method)

Baker

The Baker flow regime correlation is automatically plotted by DESIGN II when any two phase frictional pressure drop technique is specified with the exception of BEG, MUK, DUN and ORK.

Beggs Brill

Beggs and Brill calculate the flow regime and presents this information in tabular form, not as a plot.

Mukherjee Brill

The Mukherjee Brill flow regime calculation is used for all orientations of pipe and is invoked automatically when the MUKherjee Brill frictional pressure drop method is specified.

Duns Ros

The Duns Ros flow regime method is designed for vertical flow and is used when DUNs Ros frictional pressure drop method is specified. Duns Ros flow regime map is also used with the ORKiszewski pressure drop method.

Pressure Drop Due to Fluid Acceleration (default no command required)

No pressure drop due to acceleration

METHod ACCeleration

Duns Ros method to calculate pressure drop due to acceleration. The largest acceleration effect will occur where there is a significant change in velocity such as with phase changes and large overall pressure drops.

NOTE: The default print option will give the total pressure drop due to acceleration. The PRInt WIDe option in the GENeral section will show pressure drop due to acceleration for each line segment.

Line: Emulsion Commands

The Beggs Brill emulsion viscosity correction for two-liquid phase systems is available. If no emulsion command is entered, the program assumes no emulsion is formed. Tight emulsions may be encountered in pipeline flows containing between 40 and 70% water. Alternatively, an emulsion set may be specified which defines emulsion viscosities.

EMULsion = TIGHT or MEdium or LOOse or SET n

where n is the set number and the set is defined in the GENeral section.

GEN, EMULsion SET (T units) n = T,x1,r1,x2,r2,

where: T is the temperature at which the data is provided,

x are the water volume fractions

r are the corresponding viscosity ratios of emulsion to oil.

The EMUL SET command is entered in the GENeral section to specify emulsion viscosity data at different temperatures. You may enter as many sets as required. Each set may consist of data at several temperatures. By specifying the set number, that particular set will be used in a LINE module to compute the emulsion viscosity. This command can be repeated to define different temperatures and different sets.

If a set contains data at multiple temperatures, then interpolation will be performed. The program will not extrapolate. Rather, the nearest temperature data set will be used. Also any stream with water fraction larger than the last given fraction in the set will have an emulsion viscosity equal to water viscosity.

Line: Calculating Upstream Pressure

The LINE module allows a downstream pressure specification. When the down stream pressure is specified, the required upstream pressure is calculated. The calculated upstream pressure is available to other DESIGN II modules through Inline FORTRAN (see also *Line: Example Calculating Upstream Pressure*). For example, this feature may be used to specify an upstream compressor discharge pressure. The calculated upstream pressure is only reported when specified with Inline FORTRAN.

Major benefits include direct calculation of upstream pressure that achieves a given downstream pressure. Previously, an

iterative loop with a controller module was used to adjust the upstream pressure in order to achieve a specified downstream pressure and this approach can still be usefully employed in many cases.

PREssure OUT (P units) =

Example:

```

VALve 9 = V101,1,-2
      PRE OUT (PSIG) = 850
LINE 10 = P101, 2,-3
      PRE OUT (PSIG) = 350
F-    POST
F-    UPRE = GET(LINE(10),CALculated UPStream PREssure)
F-    PRINT UPRE
F-    SET(VALVE(9),PRE OUT)=UPRE
GENeral
      REC SEQ = 9,10
      MAX = 2

```

Alternately, the **CAL**culati**ON** **SEQ**uence command can be used with the **RE**peat command instead of the **REC**ycle **SEQ**uence command with **MAX**imum loops.

For Information on retrieving and printing calculated values such as upstream pressure, see *Inline Fortran: Table 2. Flowsheet Parameters Available to GET and SET*.

Line: Slug Flow Analysis

When a slug or plug flow regime is encountered, a slug flow report is printed automatically in the NOW CALLING section of your output, (appearing immediately after the pressure drop and heat transfer results).

The slug size analysis uses empirical correlations based on studies of Prudhoe Bay data (References 8,9). Based on these correlations, which include statistical analysis, the following key variables are reported in the output:

Slug length - Liquid volume of slugs in each segment
Slug velocity - Liquid holdup volume/total holdup volume
Frequency of slugs

Line: General Section Plot Commands

Plotting **LINE** Module Results

Several different **PLOT** commands for one or more **LINE** modules may be used in the same run. Each **PLOT** command will generate a separate plot.

PLOT *var1* against length for **LINE** = i1, i2, i3,....

Var 1 is a keyword from **Line: Variables Available to PLOT command**. The i1, i2, i3, etc., are the equipment numbers of **LINE** modules connected in series on the flowsheet. If multiple **LINE** module numbers are entered, the length used in the plot is the cumulative length from the start of the first **LINE** to the end of the last **LINE**.

OR

PLOT *var1 AND var2* against length for **LINE** = i1, i2, i3,....

Var 1 and *var 2* are keywords from **Line: Variables Available to PLOT command**. The i1, i2, i3, etc., are the equipment numbers of **LINE** modules connected in series on the flowsheet. If multiple **LINE** module numbers are entered, the length used in the plot is the cumulative length from the start of the first **LINE** to the end of the last **LINE**.

NOTE: The **PLOT** command belongs in the **GEN**eral section.

Line: Variables Available to PLOT command

DELta p **ELE**vation
DELta p **FR**iction
ELEvation
HOLdup

PREssure
TEMperature
VELocity

Line Pressure Drop Command Summary

Major Specifications

nominal **DI**Ameter (L units) =
INSide diameter (L units) =
LENgth of line sections (L units) =

Elevation Change Command

ELEvation (L units) =

Equivalent Length Command

EQUivalent length (L units) =

Wall Thickness Command

Calculation Method Option Commands

METHod for **FR**iction pressure drop =

Single Phase

DARcy-Weisbach

Gas Phase

American **Gas** Association

WEYmouth

PANhandle A

MODified Panhandle

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PIPE WALL thickness code =

Flow Direction Commands

HORizontal

UP

DOWN

Pipe Transport Efficiency Commands

(For gas-phase calculations)

ROUghness (L units) =

DRAg factor =

pipeline EFFiciency =

Phase Commands

SET PHase of calculation =

Segment Commands

SEGment LENGth (L units) =

SEGment ELEvation (L units) =

Liquid Holdup Calculation Method

METHod for HOLdup=

HUGHmark

DUKler

EATon

HUGHmark and PREssburg

Temperature Calculation Method Commands

TEMperature of SURroundings (T units) =
and

U (U units) =

ISOthermal

ADlabatic

Two-Phase

LOCKhart Martinelli

ORKiszewski

BEGgs and Brill

DUKler

Friction Factor Calculation Method

METHod for friction FACTor =

Single or Two-Phase

MOOdy

JAIIn

Gas Phase

AGA

WEYmouth

PANhandle A

Elevation Change Pressure Drop Calculation

METHod for ELEvation =

Gas Phase

AGA

Two-Phase

PHase density

FLAnigan

ORKiszewski

General Section PLOt Commands

PLOT variable 1 versus length for line = i₁, i₂, i₃ ...

PLOT var1 ANDvar2 versus length for line = i₁, i₂, i₃ ...

Emulsion Commands

EMULsion = TIG, MED, OR LOO

Line Pressure Drop Step by Step

Line Pressure Drop STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

LINE

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in Number

Specify one only

Line Pressure Drop STEP 2

Specify pipeline diameter and node length. More than one diameter, separated by commas, can be entered with each diameter being treated as a SEPARATE CASE.

Pipeline diameter specification (enter ONE of the following):

Nominal pipe diameter(s)

Specified inside pipe diameter

DIA (L units) =

INS (L units) =

Enter the length of line from node to node

Length of each section of line from node to node separated by commas

LEN (L units) =

Line Pressure Drop STEP 3

Choose any of the optional transmission line specification listed below.

Pipeline elevation changes option.

Net elevation change for each line node relative to the previous node (number of values must equal number entered in the LENGth command; - indicates a decrease in elevation and + indicates an increase; default is zero if no ELEvation command is entered for a HORizontal line; for a vertical (UP or DOWN) line, default is the length of line)

ELE (L units) =

Equivalent length of bends and fittings

Equivalent length of bends and fittings for each section of line from node to node (values will be added to the actual length for calculations and the number of entries must equal number of

EQU (L units) =

entries in the LENgth command

Pipe wall thickness specification (select ONE of the following)

- Standard wall (default)
- Extra strong wall
- Double extra strong wall

PIP WAL = STD
PIP WAL = XS
PIP WAL = XXS

Line flow direction specification (select ONLY ONE of the following)

- Horizontal flow (includes inclined horizontal flow)
- Vertical upwards flow (includes inclined upwards flow)
- Vertical downwards flow (includes inclined downwards flow)

HORI
UP
DOWN

Pipe roughness factor specification

- Absolute pipe roughness, or effective roughness if using the AGA friction pressure drop (L units) = default is 0.00015 feet)

ROU

Drag factor specification for the AGA pressure drop equation

- Drag factor fraction for use in the AGA equation (default is 1.0; used whenever MET FRI = AGA)

DRA = fraction

Pipeline efficiency factor specification

- Fractional pipeline efficiency for use in the Panhandle A, Modified Panhandle, and Weymouth equations (default is 1)

EFF = fraction

Line segment phase specification (select ONE of the following)

- Liquid (vapor mole fraction must be under 0.10; default is the predicted phase at each node)
- Vapor (liquid mole fraction must be under 0.10; default is the predicted phase at each node)

SET PHA = LIQ
SET PHA = VAP

Maximum length or elevation allowable per node

- Maximum segment length per node
- Maximum segment elevation per node

SET LEN (L units) =
SEG ELE (L units) =

Line Pressure Drop STEP 4

Choose any of the optional calculation method commands listed below.

Pressure drop due to friction calculation method (select ONE of the following)

- Darcy-Weisbach (default for single phase gas or liquid)
- Lockhart Martinelli (default for two-phase horizontal)
- Orkiszewski (default for two-phase vertical)
- AGA (American Gas Association)
- Weymouth
- Panhandle A
- Modified Panhandle
- Dukler (two-phase systems only)
- Beggs and Brill (two-phase systems only)

MET FRI - DAR
MET FRI = LOC
MET FRI = ORK
MET FRI = AGA
MET FRI = WEY
MET FRI = PAN
MET FRI = MOD
MET FRI = DUK
MET FRI = BEG

NOTE: Beggs and Brill cannot be combined with any other pressure drop or holdup correlations. If MET FRI = BEG is selected, all pressure drop and holdup correlations listed in Step 4 automatically default to Beggs and Brill.

Friction factor calculation method (select ONE of the following)

- Moody (default for single and two-phase flow)
- Jain
- Gas Phase Methods
 - AGA (default if MET FRI = AGA)
 - Weymouth (default if MET FRI = WEY)
 - Panhandle (default if MET FRI = PAN)

MET FAC - MOO
MET FAC = JAI

MET FAC = AGA
MET FAC = WEY
MET FAC = PAN

Method of pressure drop due to elevation change (select ONE of the following)

- Phase density (default method for both single and two-phase flow)
- Flanigan
- Gas Phase methods - AGA (default if MET FRI = AGA)
- Two-Phase methods - Orkiszewski

MET ELE = PHA
MET ELE = FLA
MET ELE = AGA
MET ELE = ORK

Liquid holdup calculation method (select ONE of the following)

- Hughmark (default)
- Dukler
- Eaton
- Hughmark and Pressburg

MET HOL = HUG
MET HOL = DUK
MET HOL = EAT
MET HOL = HUG PRE

Select one of the following options for two-liquid phase systems. (default assumes no emulsion is formed).

- tight emulsions
- medium emulsions
- loose emulsions

EMUL = TIG
EMUL = MED
EMUL = LOO

Chapter 22

Temperature calculation method (select ONE of the following options)

Option 1: Isothermal calculations (no temperature change; default)

Option 2: Adiabatic calculations

Option 3: If heat transfer option then enter both of the following options

- Temperature of the surroundings (must have same number of entries as the LENGth command)
- Overall heat transfer coefficient (must have same number of entries as the LENGth command)

ISO

ADI

TEM SUR (T units) =

U (U units) =

IF thermo is different from global (GENeral section) options THEN select

K-value option

Enthalpy option

Density option

KKE =

HKE =

DKE =

Additional output commands (enter ANY of the following options)

Plot variable 1 against length for lines i1, i2, i3 ... (where i1, i2, i3, etc., are the equipment numbers of LINE modules; command belongs in the GENeral section)

Plot variable 1 and variable 2 against length for line i1, i2, i3,... (where i1, i2, i3, etc., are the equipment numbers of LINE modules; command belongs in the GENeral section)

Variables available for these plots are:

- Elevation
- Pressure
- Delta pressure from elevation change
- Delta pressure from friction
- Holdup
- Temperature
- Velocity

PLO var1 LINE = i1, i2, i3,...

PLO var1 AND var2 LINE =
i1, i2, i3,...

ELE

PRE

DEL ELE

DEL FRI

HOL

TEM

VEL

NOTE: Each defined LINE may be plotted separately. Multiple LINEs must be in calculation order. Cumulative length will be used.

Line Pressure Drop Examples

There are several sample flowsheets in "Chapter 27: Line Module Samples - c:\designii\samples\equipmnt\line" of the DESIGN II for Windows Tutorial and Samples Guide.

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Chapter 23: LNG Exchanger

The LNG module is used to specify heating or cooling of up to twenty tubeside streams and twenty shellside streams. Each tubeside stream can have either the same outlet specification or entirely different specifications. Tubeside outlet streams may be recycled back and mixed with a single shellside feed.

LNG Exchanger Command Details

LNG Exchanger: Conventions

Coding Streams

The order in which all streams are coded for the LNG module is as follows:

- Recycle tubeside streams coded as first input and first output streams.
- Remaining tubeside streams are coded next.
- Shellside stream(s) are coded as last input and last output stream(s).

Order of Data Entries

When entering data separated by commas on one command, be sure the data for each tubeside stream is entered in the same order as the stream numbers are listed after the Equipment Module Identifier. For example, if the pressure drop for streams 8 and 10 is 5 PSIA, and 10 PSIA for streams 9 and 11, the DEL command is coded as follows:

```
LNG 3 = REFG, 8, 9, 10, 11, 30, -12, -13, -14, -15, -31
DELta pressure TUBe= 5, 10, 5, 10
```

LNG Exchanger: Tubeside Outlet Stream Specification Commands

RECYcle STREAM =

Enter the total number of tubeside streams that are to be recycled to the shellside feed. Default is zero.

Decide whether you want to use the same type of specification for all tubeside streams or use different specification types. Then, select the specification(s) from the appropriate list of commands. If you use different specification types for tubeside streams, make sure a specification command is entered for each tubeside stream. Each tubeside stream is identified by a number *n* which is the position of that tubeside stream number in the list of stream numbers following the Equipment Module Identifier. For example:

```
LNG 3 = CHIL, 10, 11, 12, 13, 20, -14, -15, -16, -17, -21,
TEMperature OUT 3 = 30
```

The command "TEMperature OUT 3 = 30" specifies the third tube stream, stream number 12, to exit at 30F (as stream number 16).

Also, make sure your specification is realistic. Be especially aware of heat transfer constraints. For example, you cannot heat a stream to a temperature higher than that of the hot streams.

If you have chosen a specification for the shellside stream(s), you cannot use any specifications for the tubeside streams.

Same Specification Used For All Tubeside Streams (enter only one)

TEMperature OUT (T units) =

Enter desired outlet temperatures, separated by commas, for tubeside streams.

TEMperature APProach (T units) =

Enter absolute temperature differences, separated by commas, between tubeside outlet streams and shellside feed.

SIMple exchanger

AREa and U for each tubeside stream are used to calculate the outlet temperatures out.

DUTy (H units/t units) =

Enter duty separated by commas, for each tubeside stream (- for cooling, + for heating).

TEMperature OUT is BUBble point

This command specifies the tubeside streams are to exit at their bubble point temperatures.

TEMperature OUT is DEW point

This command specifies the tubeside streams are to exit at their dew point temperatures.

Different specification used for tubeside streams (enter one command for each tubeside stream)

TEMperature OUT (T units) *n* =

Enter the desired outlet temperature of the *n*th tubeside stream, where *n* is its position in the list of tubeside streams following the Equipment Module Identifier.

TEMperature APProach (T units) *n* =

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Enter the desired absolute temperature difference between the nth tubeside outlet stream and the shellside feed, where n is its position in the list of tubeside streams following the Equipment Module Identifier.

DUTy (H units/t units) **n** =

Enter the desired duty for the nth tubeside stream (- for cooling, + for heating), where n is its position in the list of tubeside streams following the Equipment Module Identifier.

TEMperature **OUT** is **BUB**ble point for **n**

This command specifies the nth tubeside stream is to exit at its bubble point temperature, where n is its position in the list of tubeside streams following the Equipment Module Identifier.

TEMperature **OUT** is **DEW** point for **n**

This command specifies the nth tubeside stream is to exit at its dew point temperature, where n is its position in the list of tubeside streams following the Equipment Module Identifier.

LNG Exchanger: Shellside Streams Specifications

Multiple Shellside Streams

If more than one shellside stream is coded, the **SHELL STReam** command must be entered. Also, no mixing (recycling) of tubeside streams to shellside streams is allowed when more than one shellside stream is coded.

SHELL STReams =

Enter the number of shellside streams. Default is 1.

Specification Commands for Shellside Streams (enter only one)

If you choose a specification for the shellside stream(s), you cannot enter any specifications for the tubeside streams.

TOTAL DUTy shell (H units/t units) =

Enter one value for the duty transferred by the shellside streams.

TEMperature **OUT** of **SHELL** (T units) =

Enter only one value; all shellside streams exit at the same temperature. Tubeside streams will also exit at a single temperature.

LNG Exchanger Optional Command Details

LNG Exchanger: Heat Transfer Commands

U (U units) =

Enter the overall heat transfer coefficients, separated by commas, for each tubeside stream. Default is 50 BTU/HR/FT²/F (0.1577 KJ/SEC/M²/K . Required for SIMple exchanger.

LNG Exchanger: Pressure Drop Commands

DELta pressure of **TUB**es (P units) =

Enter the pressure drops, separated by commas, for the tubeside streams. Default is zero.

DELta pressure of **SHELL** (P units) =

Enter the pressure drop for shellside stream(s) in order and separated by commas. Default is zero.

LNG Exchanger: Geometry Commands

AREas (L² units) =

Enter the desired area-per-shell for each tubeside stream. Required for the SIMple exchanger. Default is 100 FT² (9.29 M²).

SHELLs =

Enter the number of shells. Default is 1.

SHELL PASses =

Enter the number of shell passes per shell. Default is 1.

TUBe **PAS**ses =

Enter the number of tube passes per shell. Default is 1.

LNG Exchanger: Additional Output Commands

Duty versus temperature curves for composite hot and cold streams can be obtained from the LNG Exchanger module. Multiple streams for either the shell or tube side will be summed to present a composite hot stream versus a composite cold stream. The results, presented in both tabular and graph form, indicate all critical information such as narrow temperature approach, temperature crossovers, and discontinuity in composite curves. These curves are calculated based on end-point temperature results. Bubble points, dew points, minimum approach temperature, and temperature crosses are marked on the tabular output when applicable. Example 6. Q-T Diagram contains sample results.

Q-T

Enter the keyword command.

MINimum TEMperature APProach (T units) =

Used only with the Q-T command. Enter a minimum temperature of approach value. The first point where the approach temperature falls below this value will be marked with the label MN in the Q-T tabular output.

LNG Exchanger Command Summary

Tubeside Outlet Stream Specification Commands

RECycle **ST**ream =
TEMperature **OU**T (T units) =
TEMperature **AP**Proach (T units) =
SIMple exchanger
DUTy (H units/t units) =
TEMperature **OU**T is **BUB**ble point
TEMperature **OU**T is **DEW** point
TEMperature **OU**T (T units) **n** =
TEMperature **AP**Proach (T units) **n** =
DUTy (H units/t units) **n** =
TEMperature **OU**T is **BUB**ble point for **n**
TEMperature **OU**T is **DEW** point for **n**

Shellside Streams Specifications

SHell **ST**reams =
TOTal **DU**Ty shell (H units/ t units) =
TEMperature **OU**T of **SH**ell (T units) =

Heat Transfer Commands

U (U units) =

Pressure Drop Commands

DELta pressure of **TUB**es (P units) =
DELta pressure of **SH**ells (P units) =

Exchanger Geometry Commands

AREas (L2 units) =
SHells =
SHell **PAS**ses =
TUBe **PAS**ses =

Additional Output Commands

Q-T
MINimum **TE**Mperature **AP**Proach (T units) =

Thermodynamics Commands

HKEy =
KKEy =
DKEy =

LNG Exchanger Step by Step

LNG Exchanger STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
 Equipment number
 Equipment name
 Inlet stream
 Outlet streams

LNG
 Assigned equipment flowsheet number
 User choice - up to 16 characters
 Maximum of twenty (See rules in Step 2)
 Maximum of twenty - must match number of inlet streams (See rules in Step 2)

LNG Exchanger STEP 2

Specify inlet and outlet streams. Code the inlet and outlet streams by the following rules:

- Code tubeside recycle stream(s), if any, as the first input and output stream(s)
- Code remaining tubeside stream(s)
- Code shellside stream(s) as last input and last output stream(s)

LNG Exchanger STEP 3

Choose tubeside specifications. Tubeside stream(s) recycled to the shellside feed specification.

Tubeside stream(s) recycled to the shellside feed specification

Number of tubeside outlet streams recycled to shellside inlet (no recycle streams are allowed if more than one shell stream is coded; default is zero)

REC STR =

Identical tubeside stream(s) specifications (enter ONE of the following 6 options)

Outlet temperatures, separated by commas, in order for each tubeside stream
 Absolute temperature differences, separated by commas, between each tubeside stream and shellside feed
 Simple exchanger (tubeside stream temperatures are calculated from specified AREa and U)
 Enthalpy change, separated by commas, for each tubeside stream (- for cooling, + for heating)
 Set temperatures of tubeside outlet stream(s) to their bubble points
 Set temperatures of tubeside outlet stream(s) to their dew points

TEM OUT (T units) =
TEM APP (T units) =

SIM

DUT(H units/t units) =

TEM OUT BUB
TEM OUT DEW

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IF SIMple exchanger THEN enter BOTH of the following specifications

Heat transfer area per shell (default is 100 FT SQ)

Overall heat transfer coefficients, separated by commas, in order for each tubeside stream (default is 50 BTU/HR/FT2/degrees F)

ARE (L units) =

U (U units) =

Different tubeside stream(s) specifications (enter ONE for EACH stream)

Outlet temperature of the nth tubeside stream, where n is its position in the list of tubeside streams following the Equipment Module Identifier

TEM OUT (T units) **n** =

Absolute temperature difference between the nth tubeside stream and the shellside feed, where n is its position in the list of tubeside streams following the Equipment Module Identifier

TEM APP (T units) **n** =

Enthalpy change for the nth tubeside stream (- for cooling, + for heating), where n is its position in the list of tubeside streams following the Equipment Module identifier

DUT (H units/t units) **n** =

Set temperature of the nth tubeside outlet stream to its bubble point temperature, where n is its position in the list of tubeside streams following the Equipment Module Identifier

TEM OUT BUB **n**

Set temperature of the nth tubeside outlet stream to its dew point temperature, where n is its position in the list of tubeside streams following the Equipment Module Identifier

TEM OUT DEW **n**

LNG Exchanger STEP 4

Choose shellside specification. Enter the number of shellside streams (required if more than one shell stream)

Number of shellside streams (default is 1)

SHE STR=

Shellside stream specifications (enter ONE of the following two specifications)

Enthalpy transferred by the shellside stream(s) (enter only one value; if a value is entered here, no tubeside specifications are allowed)

TOT DUT (H units/t units) =

Shellside stream(s) outlet temperature (all streams will exit at the same temperature; if a value is entered here, no tubeside specifications are allowed)

TEM OUT SHE (T units) =

LNG Exchanger STEP 5

Choose any of the optional specifications listed below:

Tubeside stream(s) pressure drops, separated by commas, in order for each tubeside stream (default is zero)

DEL TUB (P units) =

Shellside stream(s) pressure drops, separated by commas, in order for each stream (default is zero)

DEL SHE (P units) =

Number of parallel shells (default is 1)

SHE =

Number of shell passes per shell (default is 1)

SHE PAS =

Number of tube passes per shell (default is 1)

TUB PAS =

Overall heat transfer coefficients, separated by commas, in order for each tubeside stream (default is 50 BTU/HR/FT2/degrees F)

U (U units) =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

LNG Exchanger STEP 6

Choose any of the additional output information options listed below:

Duty-temperature curve keyword

Q-T

Used only with the Q-T command. Enter a minimum temperature of approach value. When the approach temperature falls below this value, the point of occurrence will be labeled with the marker "MN" on the tabular output

MIN TEM APP (T units) =

LNG Exchanger Examples

There are several sample flowsheets in "Chapter 28: LNG Exchanger Samples - c:\designii\samples\equipmnt\lngexc" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 24: Mass Balance

The MASS BALANCE module is used for setting the flowrate of a recycle loop at a certain point and / or calculating the required makeup flowrates for certain components for a recycle loop. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed stream pressure. Only one outlet stream is allowed for the module.

The components entering and leaving the flowsheet can be balanced & a specific feed stream can be assigned as a make-up stream. The feed stream to be varied by the makeup calculations of Mass Balance module can be attached to the Mass Balance module or any other module in the flowsheet. These are useful in amine contacting and glycol dehydration simulations.

Mass Balance Command Details

Mass Balance: Recycle Flowrate Commands

RECYcle flowrate (Q/t units) =

Enter the flowrate to be set for the output stream. This command is optional. No Default.

RECYcle **FLOW**rate by **COM**ponent (Q/t units) =

Enter the recycle flowrate by component to be set for the output stream. This command is optional. No Default. This command should be used separately and should not be specified in addition to the overall recycle flowrate command above.

Mass Balance: Recycle Makeup Commands

ACCeleration Factor =

Enter the acceleration factor to be used for calculating the delta change for the recycle makeup flowrate. The default is 1.0. A typical value for this command might be in the range 0.5 to 1.0, usually 1.0 or 0.8. This command is optional.

INPut Streams =

Enter the numbers of the feed streams, separated by commas, to be used for calculating the recycle makeup flowrate to be set for the varied feed stream. To use all feed streams for the flowsheet, enter -1. This command must be entered in order to calculate the recycle makeup flowrate.

OUTput Streams =

Enter the numbers of the output streams, separated by commas, to be used for calculating the recycle makeup flowrate to be set for the varied feed stream. To use all output streams for the flowsheet, enter -1. This command must be entered in order to calculate the recycle makeup flowrate.

VARy Stream =

Enter the number of the feed stream for its flowrate to be varied with the calculated recycle makeup flowrate. This command must be entered in order to calculate the recycle makeup flowrate. This stream does not have to be connected to the mass balance module.

component **IDS** =

Enter the id numbers of the component to be included in the recycle makeup flowrate calculation. Only components that are being lost to the recycle (like water, MEA, DEA, MDEA, etc...) should be part of the makeup flowrate calculation. This command must be entered in order to calculate the recycle makeup flowrate.

Mass Balance Command Summary

Major Specifications

RECYcle flow rate (Q/t units) =

RECYcle **FLOW**rate by **COM**ponent (Q/t units) =

ACCeleration factor =

INPut streams =

OUTput streams =

VARy stream =

component **IDS** =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Mass Balance Step by Step

Mass Balance STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet streams

Outlet streams

MAS BAL

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

One

Mass Balance STEP 2

Enter the flowrates for the output stream, if desired.

Output flowrate (default is lbmol/hr)

REC (Q/t units) =

OR

Enter the output recycle component flowrate (default is lbmol/hr) required

REC FLO COM =

Mass Balance STEP 3

Enter the parameters to calculate the makeup flowrate for a recycle, if desired.

Acceleration factor (default is 1.0)

ACC =

Input Stream numbers for the recycle feeds (-1 for all feed streams in the flowsheet) (must be specified for calculation)

INP =

Output Stream numbers for the recycle products (-1 for all product streams in the flowsheet) (must be specified for calculation)

OUT =

Varied feed Stream number (must be specified for calculation)

VAR =

Component IDs (must be specified for calculation)

IDS =

If thermo is different from global (GENeral section) options THEN select:

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Mass Balance Examples

There are several sample flowsheets in "Chapter 29: Mass Balance Samples - c:\designii\samples\equipmnt\masbal" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 25: Mixer

The MIXer is a single-purpose module that is used to mix multiple input streams. The feed streams are adiabatically flashed to the lowest inlet stream pressure. Since most DESIGN II Equipment Modules accept an essentially unlimited number of input streams and adiabatically mix them before calculation, the MIXer is seldom required for flowsheet simulation.

The advantage of using the MIXer with a two phase outlet stream is that the properties of the mixed stream are reported in the printout. This is not the case in modules which automatically mix multiple feeds and then proceed with calculations.

If two outlet streams are coded, the module performs a phase separation of the mixed stream. The vapor portion is placed in the first outlet stream, the liquid in the second. Note that this applies only for the old input file management cases. On flowsheet process flow diagram, and when you are not interested in the mixed output stream you can use one of the following Equipment Modules thereby eliminating the MIXer module.

FLash, **VAL**ve, **COM**ponent **SPL**itter, **PUM**p, **COM**pressor, **REA**ctor, **DIS**tillation, **REF**ine, **DIV**ider, **SHO**rtcut fractionator, **EXP**ander, **ST**ream manipulator, **FIR**ed heater, and **LINE**.

If you are not interested in the mixed output stream and are using one of the following Equipment Modules, you can eliminate the MIXer:

COMponent **SPL**itter
COMpressor
DIStillation
DIVider
EXPander

FIRed heater
FLash
LINE
MASs BALance
PUMp

REFine
SHOrtcut fractionator
STream manipulator
REActor
VALve

Mixer Command Details

No input/output specifications are available for the MIXer module.

Mixer Optional Command Details

PREssure **OUT** (P units) =

This is an optional command. Enter desired discharge pressure.

Notes:

If the outlet pressure is not specified then the outlet pressure will be set to the lowest pressure of the incoming feed stream(s) with non-zero flowrate.

The outlet pressure cannot be set higher than the highest of the incoming feeds pressure.

Mixer Command Summary

Required Commands

Must enter the numbers of the flowsheet streams to be mixed (unlimited) and the number(s) of the flowsheet stream(s) representing the mixer outlet(s).

Optional Commands

PRE OUT (P units) =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Mixer Step by Step

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

MIX

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

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Outlet streams

One or two; 1st is vapor, 2nd is liquid

No further input specifications are required for the MIXer module

Enter optional command, if desired.

Enter the output pressure required

PRE OUT =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Mixer Examples

There are several sample flowsheets in "Chapter 30: Mixer Samples - c:\designii\samples\equipment\mixer" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 26: Multiple Flashes

The MULTiple FLAsh module can perform isothermal, adiabatic, isentropic, liquid fraction (molar or mass), bubble point, dew point, and water dew point calculations. Either temperature or pressure can be specified for the above options. Heat addition/removal can be included for adiabatic flash calculations. An isothermal flash is the default option.

One inlet stream can be flashed up to fifty times or up to fifty separate inlet streams can be flashed. No phase separation will be performed, but the phase information will be contained in the detailed stream summaries. If phase separation is required for any outlet stream, use a VALve or FLAsh module.

Multiple Flashes Optional Command Details

Multiple Flashes: Stream Guidelines

Two options are available for stream input in the MULTiple FLAsh module. You can have one inlet stream and up to 50 outlet streams (all same composition and flow as inlet stream) or up to fifty inlet streams and an equal number of outlet streams. Specifications and calculation options always refer to outlet stream numbers, not inlet stream numbers.

The default calculation option is an isothermal flash. If no TEMperature OUT and/or PREssure OUT command is used, the flash will be performed at the inlet temperature and pressure for the stream. For all flashes other than isothermal, you can specify either the temperature or the pressure out. The program will then solve for the corresponding pressure or temperature. If both TEMperature OUT and PREssure OUT are specified, PREssure OUT is treated as the specification and the TEMperature OUT command will be ignored.

Multiple Flashes: Calculation Options for Multiple Flashes

Note: j1, j2 refer to outlet stream numbers

ADIabatic = j1,j2,

Enter the outlet stream numbers which are to be flashed adiabatically.

HEAt **ADD**ed (H units/t units) = j1,specification, j2,specification

Enter the outlet stream numbers and the amount(s) of heat added to or subtracted from the flash in pairs. A negative value indicates heat subtracted from the flash.

ISEntropic =j1,j2,

Enter the stream numbers for which an isentropic flash is to be performed.

BUBble point = j1,j2,

Enter the outlet stream numbers for which bubble points are to be calculated.

DEW point = j1,j2,

Enter the outlet stream numbers for which dew points are to be calculated (hydrocarbon dewpoint for immiscible flash).

DEW WATer = j1,j2,

Enter the outlet stream numbers for which water dew points are to be calculated (IMM = 62 must be specified in GENeral section).

LIQuid **FRA**ction = j1,specification, j2,specification

Enter the outlet stream numbers and the desired molar liquid fractions in pairs.

LIQuid **FRA**ction (MASS) = j1,specification, j2,specification

Enter the outlet stream numbers and the desired mass liquid fractions in pairs.

VAPor = j1,j2,

Enter the outlet stream numbers which are to be set to the vapor phase at the inlet temperature and pressure (or at a specified temperature and pressure).

LIQuid =j1,j2

Enter the outlet stream numbers which are to be set to the liquid phase at the inlet temperature and pressure (or a specified temperature and pressure).

Multiple Flashes: Outlet Pressure and Temperature Specifications

For isothermal flashes, you may specify both outlet stream temperature and pressure. All other calculation options allow you to specify outlet stream temperature pressure. (j1, j2 represent outlet stream numbers)

PREssure **OUT** (P units) = j1,specification, j2,specification

Enter the outlet stream numbers and the desired outlet pressures in pairs.

TEMperature **OUT** (T units) =j1,specification, j2,specification

Enter the outlet stream numbers and the desired outlet temperatures in pairs.

Multiple Flashes Command Summary

Calculation Options

ADiabatic = $j_1, j_2, ..$
ISEentropic = $j_1, j_2, ..$
HEAt **ADD**ed (H units/t units) = $j_1, \text{specification}, j_2, \text{specification}, ..$
BUBble point = $j_1, j_2, ..$
DEW point = $j_1, j_2, ..$
DEW point of **W**ATER = $j_1, j_2, ..$
LIQuid **F**RAction = $j_1, \text{specification}, j_2, \text{specification}, ..$
LIQuid **F**RAction (**MAS**s) = $j_1, \text{specification}, j_2, \text{specification}, ..$
VAPor = $j_1, j_2, ..$
LIQuid = $j_1, j_2, ..$

Outlet Pressure and Temperature

Specifications

PREssure **OUT** (P units) = $j_1, \text{specification}, j_2, \text{specification}, ..$
TEMperature **OUT** (T units) = $j_1, \text{specification}, j_2, \text{specification}, ..$

Thermodynamics Commands

HKEy =
KKEy =
DKEy =

Multiple Flashes Step by Step

Multiple Flashes STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
 Equipment number
 Equipment name
 Inlet stream
 Outlet streams

MUL FLA

Assigned equipment flowsheet number
 User choice - up to 16 characters
 Up to fifty
 Up to fifty

NOTE: Up to 50 outlet streams can be coded for a single inlet stream. The number of outlet streams must equal the number of inlet streams if multiple inlet streams are coded.

Multiple Flashes STEP 2

OPTIONAL - Choose any of the optional outlet stream specifications listed below. Select ONE only.

NOTE: Isothermal flash needs both temperature and pressure specifications. Otherwise, DESIGN II will use the inlet temperature and pressure. For isentropic and adiabatic flashes both temperature and pressure need not be specified. If both are specified, temperature will be varied.

Adiabatic flash
 Specified heat addition

Isentropic flash
 Streams for which bubble points are to be calculated (same as LIQ FRA = 1)
 Streams for which the dew points are to be calculated (same as LIQ FRA = 0)
 Streams for which the dew points are to be calculated (IMM = 62 must be specified in the GENeral section)
 Specified molar liquid fractions for outlet stream

Specified mass liquid fraction for outlet stream

Outlet streams specified as vapor phase
 Outlet streams specified as liquid

Outlet pressure and temperature specifications (select ONE of the following)

Pressure out for each outlet stream

Temperature out for each outlet stream

ADI = $j_1, j_2, ..$
HEA ADD (H units/t units) = $j_1, \text{specification}, j_2, \text{specification}, ..$
ISE = $j_1, j_2, ..$
BUB = $j_1, j_2, ..$
DEW = $j_1, j_2, ..$
DEW WAT = $j_1, j_2, ..$

LIQ FRA = $j_1, \text{specification}, j_2, \text{specification}, ..$
LIQ FRA (MASs) = $j_1, \text{specification}, j_2, \text{specification}, ..$
VAP = $j_1, j_2, ..$
LIQ = $j_1, j_2, ..$

PRE OUT (P units) = $J_1, \text{specification}, j_2, \text{specification}, ..$
TEM OUT (T units) = $j_1, \text{specification}, j_2, \text{specification}, ..$

NOTE: For isothermal flashes both PRE OUT and TEM OUT may be specified. If you do not specify temperature and pressure, the inlet conditions will be used as needed. In the event of over-specification, temperature will be varied.

IF thermo is different from global (GENeral section) options THEN select

K-value option
 Enthalpy option
 Density option

KKE =
HKE =
DKE =

Multiple Flashes Examples

There are several sample flowsheets in “Chapter 31: Multiple Flashes Samples - c:\designii\samples\equipmnt\mulflash” of the DESIGN II for Windows Tutorial and Samples Guide.

Multiple Flashes: With a ChemTran File

```
*MULTIFLASH WITH CHEMICAL FILE
MULTiple FLAsh 50 = DUMMY, 1, -2, -3, -4, -5,-6,
    DEW point = 6,
    BUBble point = 2,
    ADIabatic = 3,
    TEMperature OUT = 4, 170,
    HEAt addition (KCAL/HR) = 5, 1.5E6
GENeral
    COMponents = 1, 2, 22, 3, 66, 23, 4
    FLOW (KGMOL/HR) 1 = 1.7637, 3.0865, 2029.1,
    798.65,1000, 275.389, 450
    TP 1 = -9.6655, 281.8
    CHEmical FILE = PENG, DATA, FILE
    PENK, COPE
END
```

Multiple Flashes: Constructing Bubble and Dew Point Curves

(From the DESIGN II Menu Bar, please select...Simulate...Use Existing Files...
c:\designii\samples\equipmnt\mulflash\mulfla3.in to simulate this problem)

The output from this example can be used to construct a vapor-liquid equilibrium curve

```
*DEW POINT CURVES, BUBBLE POINT CURVES
MULTiple FLAsh 10 = BUB, 1, 2, 3, 4, 5, 6, 7,8, 9, 10, 11,
    12, 13, 14, 15, 16, 17, 18, 19, 20, 21, -22, -23, -24,
    -25, -26, -27, -28, -29, -30, -31, -32, -33, -34,
    -35, -36, -37, -38, -39, -40, -41, -42,
    BUBble point = 22, 23, 24, 25, 26, 27, 28, 29, 30,31,
    32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42,
    KKE=SOAVEK, HKE=COPE,
MULTiple FLAsh 11 = DEW, 51, 52, 53, 54, 55, 56, 57, 58, 59,
    60, 61, 62, 63, 64, 65, -66, -67, -68, -69, -70,
    -71, -72, -73, -74, -75, -76, -77, -78, -79, -80,
    DEWpoint = 66, 67, 68, 69, 70, 71, 72, 73, 74, 75,76,
    77, 78, 79, 80,
    KKE = PENK
    HKE = COPE
GENeral
    COMponents = 2, 3, 49, RKK
    FLOW 1 = .0265, .4432, .5303, TP (K, ATM) 1 = 250, 21
    FLOW 2 = .1728, .5700, .2572, TP (K, ATM) 2 = 250, 21
    FLOW 3 = .1602, .5615, .2783, TP (K, ATM) 3 = 250, 21
    FLOW 4 = .2500, .6200, .1300, TP (K, ATM) 4 = 250, 21
    FLOW 5 = .0288, .2007, .7715, TP (K, ATM) 5 = 250, 21
    FLOW 6 = .0374, .1700, .7926, TP (K, ATM) 6 = 250, 21
    FLOW 7 = .0400, .1600, .8000, TP (K, ATM) 7 = 250, 21
    FLOW 8 = .0235, .2154, .7611, TP (K, ATM) 8 = 250, 21
    FLOW 9 = .3521, .5377, .1102, TP (K, ATM) 9 = 250, 25
    FLOW 10= .3264, .5264, .1472, TP (K, ATM) 10 = 250, 25
    FLOW 11= .1901, .4148, .3951, TP (K, ATM) 11 = 250, 25
    FLOW 12= .1323, .2937, .5740, TP (K, ATM) 12 = 250, 25
    FLOW 13= .1387, .2601, .6012, TP (K, ATM) 13 = 250, 25
    FLOW 14= .1701, .1623, .6676, TP (K, ATM) 14 = 250, 25
    FLOW 15= .2464, .4730, .2806, TP (K, ATM) 15 = 250, 25
    FLOW 16= .4021, .4531, .1448, TP (K, ATM) 16 = 250, 30
    FLOW 17= .2605, .2845, .4550, TP (K, ATM) 17 = 250, 30
    FLOW 18= .2580, .2420, .5000, TP (K, ATM) 18 = 250, 30
    FLOW 19= .3025, .0935, .6040, TP (K, ATM) 19 = 250, 30
    FLOW 20= .2630, .2270, .5100, TP (K, ATM) 20 = 250, 30
    FLOW 21= .3448, .4182, .2370, TP (K, ATM) 21 = 250, 30
    FLOW 51= .0033, .4512, .5455, TP (K, ATM) 51 = 250, 21
    FLOW 52= .0352, .7898, .1750, TP (K, ATM) 52 = 250, 21
    FLOW 53= .0020, .1198, .8782, TP (K, ATM) 53 = 250, 21
    FLOW 54= .0022, .0986, .8992, TP (K, ATM) 54 = 250, 21
    FLOW 55= .0999, .8189, .0812, TP (K, ATM) 55 = 250, 25
    FLOW 56= .0950, .8097, .0953, TP (K, ATM) 56 = 250, 25
    FLOW 57= .0508, .5792, .3700, TP (K, ATM) 57 = 250, 25
```

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```
FLOW 58= .0298, .3158, .6545, TP (K, ATM) 58 = 250, 25
FLOW 59= .0282, .2662, .7056, TP (K, ATM) 59 = 250, 25
FLOW 60= .0247, .1392, .8361, TP (K, ATM) 60 = 250, 25
FLOW 61= .1351, .7350, .1300, TP (K, ATM) 61 = 250, 30
FLOW 62= .0705, .3741, .5554, TP (K, ATM) 62 = 250, 30
FLOW 63= .0685, .3250, .6064, TP (K, ATM) 63 = 250, 30
FLOW 64= .0520, .2495, .7085, TP (K, ATM) 64 = 250, 30
FLOW 65= .1203, .6652, .2145, TP (K, ATM) 65 = 250, 30
TEMPerature UNITS OUT = K,
PREssure UNITS OUT = ATM,
BIN PAR = PENG1
```

END

Chapter 27: Multiple Phase Flash

The MULTIPLE PHASE flash module can be used to rigorously separate multiple phase streams. One inlet and at least three outlet streams should be coded. The vapor phase is placed in the first outlet stream and the liquid phases are placed in the other outlet streams.

Multiple Phase Flash Overview

The module can be used with activity coefficient K-value options such as RENon, UNIQUAC, and UNIFAC or cubic equations of state such as PENG-Robinson K, SOAVEK, APISOAVEK, MODIFIED PENG-Robinson K, or Soave-Kabadi-Danner (SKDK). Vapor-liquid and/or liquid-liquid equilibrium data can be fitted using RENon, UNIQUAC or an equation of state. Alternately, the UNIFAC option can be used to estimate infinite dilution activity coefficients. To get the best results for a three-phase flash, you should fit either liquid-liquid equilibrium data or a combination of vapor-liquid and liquid-liquid equilibrium data to either the RENon or UNIQUAC equations.

The three-phase system parameters for these correlations are typically temperature dependent. Better results can be expected if the degree of temperature extrapolation is low. If possible, the data which is being fitted should be at operating conditions or span the operating conditions. If the data covers a wide temperature range, the temperature dependency parameter (B12) should be varied during the data regression.

NOTE: If the value of the non-randomness parameter (C12) for the RENon equation exceeds 0.426, no liquid-liquid phase splitting will be predicted. See ChemTran for commands and guidelines for fitting mixture data.

The UNIFAC group contribution technique can also be used, but it should not be considered as a substitute for experimental data. The WILSON equation should not be used for these calculations as it has no provision for predicting behavior in the partially miscible region.

An estimate of the outlet stream's phase and flowrate can be entered in the GENERAL section to provide a starting point for the MULTIPLE PHASE flash calculation. The standard two-phase stream initialization will be used as a default.

Multiple Phase Flash Command Details

There are no specifications for this module. An isothermal flash will be performed at the inlet stream temperature and pressure.

Multiple Phase Flash Optional Commands

MAXimum ITERations =

Enter the maximum number of iterations.

Multiple Phase Flash Command Summary

Optional Commands

MAXimum ITERations =

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Multiple Phase Flash Step by Step

Multiple Phase Flash STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

MUL PHA

Assigned equipment flowsheet number

User choice - up to 16 characters

One only

At least three - 1st contains vapor phase

OPTIONAL - Choose any of the optional outlet streams

Calculation and Print Options

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Maximum number of iterations (default is 30)

MAX ITE =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

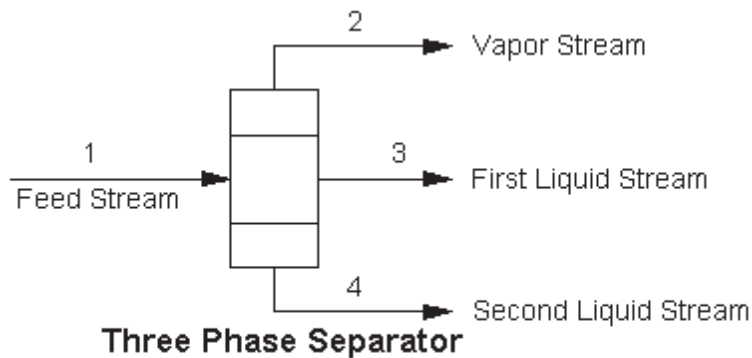
Density option

DKE =

Multiple Phase Flash Examples

There are several sample flowsheets in "Chapter 32: Multiple Phase Flash Samples - c:\designii\samples\equipmnt\mulphase" of the DESIGN II for Windows Tutorial and Samples Guide.

Multiple Phase Flash: Using Data Regressed to an Equation of State



AB123.

* Modified Peng Robinson with Margules Mixing method.

MULTiple PHase 1 = VOL,1,-2,-3,-4,

GENeral

COMPonents = 1021,62,41,3

FLOw 1 = 50,5,10,2

TP (C) 1 = 25,14.7

MOD PENK, LAT

EOS MIX = MAR

CHEmical **FILE** = MEOH,VOL,DATA

END

Chapter 28: Packed Column

The PACKed COLumn module is used for rigorous simulation of absorbers. Most single-column units can be modeled, including demethanizers, stabilizers, and sour water strippers. This module can be used for design, modification, or optimization of rigorous packed columns. Extensive thermodynamic options are available (see [Thermodynamics Section](#)). With the use of the proper option, the operation of existing units can be duplicated within several percent of actual plant data.

Packed Column Features

The PACKed COLumn module offers contact between two feeds and separation into two product streams.

This first phase of project will have:

1. Number of sections
2. HETP per section
3. Packing depth per section
4. Pressure drop per section
5. Column diameter
6. Packing height per section
7. Packing material and Packing shapes.

The second phase of this project will have (please check back here in future Versions):

An option for the column to calculate the HETP for each section using the reference Billet and Schultes, September 1999, for dumped and structured packings.

Specifications

The PACKed COLumn module allows specifications for number of sections, packing depth per section, HETP per section and pressure drop per section. When user does not know HETP data, they can provide column diameter, packing height, packing material and packing shape that calculates HETP.

Calculation Techniques

Internal convergence algorithms can be fine tuned to meet user specified tolerances and number of iterations.

Stream Order Convention

Certain conventions must be followed when defining feed and product streams in the PACKed COLumn module. These conventions are listed below:

Each feed stream to the PACKed COLumn module is assigned a unique number. The feed stream numbers are listed in top-to-bottom order.

Each product stream is assigned a unique number. The product stream numbers are given negative signs and listed in top-to-bottom order.

Packed Column Command Details

The following are required commands.

NUMBER of SECTIONS =

Enter the number of sections of the packed column. This must be the first command following PACKed COLumn, if using an input generation.

Default is none and must have value.

SECTION DEPTH (L units) =

Enter the depth of the section(s). Default is none and must have value.

HETP (L units) =

Enter the height equivalent of a theoretical plate. This must be less than SECTION DEPTH and if HETP is greater than SECTION DEPTH then the number of stages is set to one.

FEED LOCATION (L units) =

Enter the feed location distances from top of column with comma separated for multiple distances.

TOP PRESSURE (P units) =

Enter the packed column's top pressure. Default is none and must have value.

BOTTOM PRESSURE (P units) =

Enter the packed column's bottom pressure. Default is none and must have value.

Option 1: User known HETP data

SECTION DEPTH (L units) =

Enter the depth of the section(s). Default is none and must have value.

HETP (L units) =

Enter the height equivalent of a theoretical plate. This must be less than SECTION DEPTH and if HETP is greater than SECTION DEPTH then the number of stages is set to one.

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PREssure DROp per section (P units) =

Enter the pressure drop per section for the column. Default is zero.

Option 2: Calculate HETP data

COLumn DIAMeter (L units) =

Enter the diameter of the column. Default is none and must have value.

SECTion HEIght (L units) =

Enter the height of the section(s). Default is none and must have value.

and [Packed Column Material Command Details](#)

PREssure DROp per section (P units) =

Enter the pressure drop per section for the column. Default is zero.

Packed Column Optional Command Details

Packed Column: Convergence Control

TOLerance =

Enter the maximum acceptable tolerance for the column. The default is TOL = 0.1 E-5.

MAXimum ITeration =

Enter the maximum number of matrix inversions for column solution. Default is 200.

Packed Column Material Command Details

PACKing MATerial =

Enter the type of packing materials from this list: **METal** or **PLAstic** or **CERamic** or **ALUminum**. Default is none and must have value.

PACKing SHApe = number

Enter the number corresponding to the following list of packing shapes. Default is none and must have value.

Metal Packing

1	Raschig Super-Ring	0.3 mm
2	Raschig Super-Ring	0.5 mm
3	Raschig Super-Ring	1 mm
4	Raschig Super-Ring	2 mm
5	Raschig Super-Ring	3 mm
6	Pall Ring	50 mm
7	Pall Ring	35 mm
8	Pall Ring	25 mm
9	Ralu Ring	50 mm
10	Ralu Ring	38 mm
11	Ralu Ring	25 mm
12	Hiflow-Ring	50 mm
13	Hiflow-Ring	25 mm
14	Hiflow-Ring	50 mm
15	Glitsch Ring	30 PMK
16	Glitsch Ring	30 P
17	Glitsch CMR Ring	1.5"
18	Glitsch CMR Ring	1.5" T
19	Glitsch CMR Ring	1.0"
20	Glitsch CMR Ring	0.5"
21	VSP Ring	50 mm
22	VSP Ring	25 mm
23	Bialecki Ring	50 mm
24	Bialecki Ring	35 mm
25	Bialecki Ring	25 mm
26	Bialecki Ring	35 mm
27	Ralu Pak	YC-250
28	Mellapak	250Y
29	Gempack	A2T-304

30	Impulse packing	250 mm
31	Montz Packing	B1-200
32	Montz Packing	B2-300

Plastic Packing

1	Raschig Super-Ring	2 mm
2	Ralu Flow	1 mm
3	Ralu Flow	2 mm
4	Pall Ring	50 mm
5	Pall Ring	35 mm
6	Pall Ring	25 mm
7	Ralu Ring	50 mm
8	Ralu Ring	38 mm
9	Ralu Ring	25 mm
10	NOR PAC Ring	50 mm
11	NOR PAC Ring	35 mm
12	NOR PAC Ring	25 mm
13	NOR PAC Ring	25 mm
14	Hiflow-Ring	50 mm hydrophilic
15	Hiflow-Ring	50 mm S
16	Hiflow-Ring	25 mm
17	Envi Pac Ring	80 mm
18	Envi Pac Ring	60 mm
19	Envi Pac Ring	32 mm
20	Tellerette	25 mm
21	Hackette	45 mm
22	Raflux Ring	15 mm
23	DIN-PAK	70 mm
24	DIN-PAK	47 mm
25	Montz Packing	C1-200
26	Montz Packing	C2-200
27	Euroform	PN-110

Ceramic Packing

1	Hiflow-Ring	50 mm
2	Hiflow-Ring	38 mm
3	Hiflow-Ring	20 mm
4	Raschig Ring	50 mm
5	Raschig Ring	25 mm
6	Berl Saddle	25 mm
7	Berl Saddle	13 mm
8	Pall Ring	50 mm
9	Impulse Packing	100 mm

Aluminum Packing

1	TOP Pak Ring	50 mm
---	--------------	-------

Packed Column Command Summary

Required Column Description

NUMBER of **SECTIONS** =
SECTION DEPTH (L units) =
HETP (L units) =
FEED LOCATION (L units) =
TOP PRESSURE (P units) =

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BOT PREssure (P units) =
PREssure **DRO**p per section (P units) =
COLumn **DIA**meter (L units) =
SECtion **HEI**ght (L units) =
PACKing **MAT**erial = **MET**al or **PLA**stic or **CER**amic or **ALU**minum
PACKing **SHA**pe = number

Convergence Control

TOLerance =
MAXimum **ITE**ration =

Packed Column Step by Step

Packed Column STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream(s)

Outlet stream(s)

PAC COL

Assigned equipment flowsheet number

User choice - up to 16 characters

Maximum of two, in top-to-bottom order

Maximum of two, in top-to-bottom order

Packed Column STEP 2

Enter the required column description.

Required column description (enter ALL of the following).

Number of packed sections

Depth of the section

Height Equivalent of a Theoretical plate

Feed Location

Top pressure

Bottom pressure

Column pressure drop (default is 0)

Diameter of the column.

Packing section height

Packing materials

Packing shape (see [Packing Materials](#)) .

NUM SEC =

SEC DEP (L units) =

HETP (L units) =

FEE LOC (L units) =

TOP PRE (P units) =

BOT PRE (P units) =

PRE DRO (P units) =

COL DIA (L units) =

SEC HEI (L units) =

PACKing **MAT**erial = **MET**al or **PLA**stic or
CERamic or **ALU**minum.

PACKing **SHA**pe = number

Packed Column STEP 3

Enter the optional column commands.

Convergence Tolerance

Maximum number of Iterations

TOL =

MAX ITE =

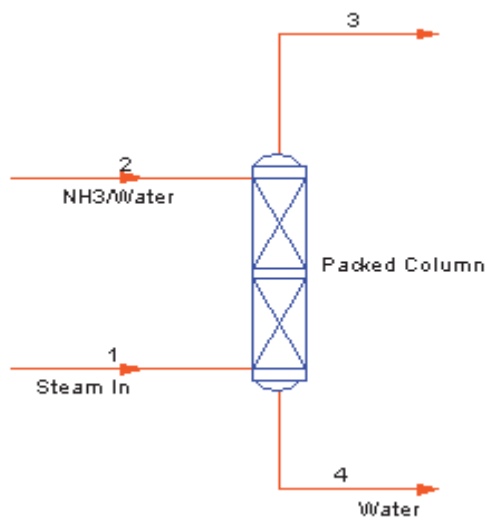
Packed Column Examples

There are several sample flowsheets in "Chapter 35: Packed Column Samples - c:\designii\samples\equipmnt\packedcolumn" of the DESIGN II for Windows Tutorial and Samples Guide.

Packed Column: Packed Column.psd - Ammonia Water Contactor

(From the DESIGN II Menu Bar, please select...File...Open...

c:\designii\samples\equipmnt\packedcolumn\Packed Column.psd to simulate this problem)



A single section packed column is simulated for stripping out NH₃ from an aqueous stream using steam.

AB123.

*

C- EQUIPMENT MODULES

PAC COL 2 = Packed Column, 2,1,-3,-4,

NUM SEC = 1

SEC DEP(FT) = 15,

HETP(FT) = 2,

TOP PRE(KPA) = 445

PRE DRO(KPA) = 1,

MAX ITE = 100

TOL = 1e-005

C- GENERAL SECTION

GENERAL

COMPONENTS = 62,63,

NAM POS 1 = 'WATER'

NAM POS 2 = 'AMMONIA'

APISOUR

LAT

STDD

DEN LIQ = STDD

SUR TEN = STD

STE TAB

PRE UNI OUT = PSIG

AME UNI OUT

MAX = 10

CON TOL = 0.001

FLO(LB/HR)1 = 1042,

TP (F,PSIG) 1 = 385,50

NAM STR 1 = Steam In

FLO(LB/HR)2 = 7934.8,365.2,

TP (F,PSIG) 2 = 239,50

NAM STR 2 = NH₃/Water

NAM STR 3 = Strm 3

NAM STR 4 = Water

END

Packed Column References

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3. Billet R., Packed Towers in Processing and Environmental Technology, 1995, ISBN 3527286160.
4. Strigle R., Packed Tower Design and Applications, 1994, ISBN 0884151794
5. Kister, Henry. Distillation Design. 1992. ISBN-0070349096.
6. Green D., Perry R., Perry's Chemical Engineers' Handbook, 8th Edition, 2008, ISBN 9780071422949
7. Poling B., Prausnitz J., O'Connell J., The Properties of Gases and Liquids, 5th edition, McGraw-Hill, 2000.
8. Fuller, E.N., and J.C. Giddings: J. Gas Chromatogr., 3: 222 (1965)
9. Fuller, E.N., P.D. Schettler, and J.C. Giddings: Ind. Eng. Chem., 58(5): 18 (1966)
10. Fuller, E.N., K. Ensley, and J.C. Giddings: J. Phys. Chem., 73: 3679 (1969)

Chapter 29: Phase Envelope

The PHase envelope module calculates dew and bubble points for specified pressures. The properties of the feed stream are passed to the output stream. Critical points are rigorously calculated using the Peng-Robinson equation of state. Binary interaction parameters will be considered if they are present. See *Calculation Options: Stream (Mixture) Properties* section for critical pressure and temperature calculations for natural gas streams.

Once the critical pressure is reached (normally on the dew point side of the envelope) further dew point calculations would be meaningless. DESIGN II will attempt to calculate bubble points to fill in the points at the top of the envelope. Similarly, if the critical is on the bubble point side, DESIGN II will attempt to calculate dew points to fill in the top of the envelope.

Phase Envelope Command Details

Phase Envelope Calculation Pressures

PREssures (P units) =

Enter up to thirty pressures, separated by commas, at which dew and bubble points are to be calculated. Zeroes entered between pressures will result in linear interpolation of pressures. For example:

PREssures = 100, 8*0, 1000

Is the same as

PREssures = 100,200,300,400,500,600, 700,800,900,1000

Pressures must be entered in increasing order.

NOTE: Do not use the interpolation feature if you are entering pressure values using gauge pressures.

Phase Envelope Temperature Guesses

TEMperature guess for **BUB**ble point (T units) =

Enter a guess for the bubble point temperature at the first pressure specified. Default is feed temperature.

TEMperature guess for **DEW** point (T units) =

Enter a guess for the dew point temperature at the first pressure specified. Default is feed temperature.

Phase Envelope Command Summary

Calculation Pressures

PREssures (P units) =

Temperature Guesses

TEMperature guess for **BUB**ble point (T units) =

TEMperature guess for **DEW** point (T units) =

Thermodynamic Commands

HKEy=

KKEy=

DKEy=

Phase Envelope Step by Step

Phase Envelope STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

PHA

Assigned equipment flowsheet number

User choice - up to 16 characters

One only

One only

Phase Envelope STEP 2

Enter up to thirty pressures for calculations

Pressures for bubble and dew point calculations (enter in increasing order; separate with commas)

PRE (P units) =

Phase Envelope STEP 3

Enter bubble and dew point temperature guesses

Bubble point guess for first pressure

TEM BUB (T units) =

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Dew point guess for first pressure

TEM DEW (T units) =

OPTIONAL - Choose any of the optional specifications listed below:

IF thermo is different from global (GENeral section) options THEN select

K-value option

Enthalpy option

Density option

KKE =

HKE =

DKE =

Phase Envelope Examples

There are several sample flowsheets in "Chapter 33: Phase Envelope Samples - c:\designii\samples\equipment\phaseenv" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 30: Phase Map

The PHase MAP module calculates dewpoints, bubble points and constant liquid fraction lines for hydrocarbon systems. This module uses improved numerical techniques to perform rigorous calculations in the entire region.

Phase Map Features

At the present time, the PHase MAP module will use only APISOAVE, SOAVE, and PENG-ROBINSON equations of state (with or without interaction parameters) for K-value calculations. PHase MAP calculations will be performed using SOAVEK when any of the following thermodynamic options are specified in the GENeral section: STDK (default), KVAL, RKK, BWRK, and BWRSK. In all cases the critical temperature and pressure are calculated with the Peng-Robinson equation of state. Lines of constant liquid fraction for 0.0 (dew point), 0.50, and 1.0 (bubble point) are automatically calculated. Output will include the critical temperature and pressure of the mixture; temperature, pressure, compressibility factor and enthalpy (in molar units) for each of the bubble and dew points calculated; and a plot of the tabulated temperature pressure points. Temperature, pressure, and compressibility factors will be reported for the other lines of constant liquid fraction.

NOTE: Three-phase water hydrocarbon streams are not allowed by the PHase MAP modules.

There are three advantages to using the PHase MAP module to generate a phase envelope for a hydrocarbon mixture: 1) more accurate prediction of temperatures and pressures for bubble points and dew points including the critical region, and 2) calculation of up to 5 lines of constant liquid fraction within the envelope (3) more efficient calculation for all the data points generated. Moderate amounts of carbon dioxide, nitrogen, and hydrogen sulfide are allowed in the hydrocarbon mixture, but absolutely **NO WATER** is allowed. Use the MULTiple FLAsh module to calculate water dew points in a water-hydrocarbon system.

Phase Map Command Details

TEMperature of **BUB**ble point (T units) =

Enter guess for the bubble point temperature at 146.96 PSIA (10 atm).

TEMperature of **DEW** point (T units) =

Enter guess for the dew point temperature at 146.96 PSIA (10 atm).

Initial **PRE**ssure of **BUB**ble point curve (P units) =

Enter the initial pressure for the bubble point curve calculations. Default is 146.96 PSIA (10 atm).

Initial **PRE**ssure of **DEW** point curve (P units) =

Enter the initial pressure for the dew point curve calculations. Default is 146.96 PSIA (10 atm).

Phase Map Optional Command Details

LIQuid **FRA**ction =

Enter the molar liquid fractions you want calculated in addition to the default value of 0.50 (maximum of 5 values, including the 0.50 line) separated by commas.

Initial **PRE**ssure (P units) =

Enter desired starting pressures, separated by commas, for liquid fraction calculations. Use only with LIQ FRA command. Must have a one-to-one correspondence with values entered in the LIQ FRA command. Default is 10 atmospheres.

TEMperature **GUE**ss (T units) =

Enter a guess for the starting temperature for each liquid fraction specified.

Phase Map Command Summary

Temperature Guesses

TEMperature of **BUB**ble point (T units) =

TEMperature of **DEW** point (T units) =

Initial Pressures

Initial **PRE**ssure of **BUB**ble point curve (P units) =

Initial **PRE**ssure of **DEW** point curve (P units) =

Optional Specifications

LIQuid **FRA**ction =

TEMperature **GUE**ss (T units) =

INItial **PRE**ssure (P units) =

Thermodynamic Commands

HKEy=

KKEy=

DKEy=

Phase Map Step by Step

Phase Map STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

PHA MAP

Assigned equipment flowsheet number

User choice - up to 16 characters

One only

One only

Phase Map STEP 2

Enter bubble and dew point temperature guesses

Guess for bubble point temperature at initial pressure

Guess for dew point temperature at initial pressure

TEM BUB (T units) =

TEM DEW (T units) =

Initial pressure for bubble point curve calculations

Initial pressure for dew point curve calculations

PRE BUB (P units) =

PRE DEW (P units) =

OPTIONAL - Choose any of the optional specifications listed below:

Molar liquid fractions to be calculated in addition to 0.5 (maximum of five, including 0.5)

Starting temperature guess for each fraction specified

Starting pressure for each liquid fraction specified

LIQ FRA =

TEM GUE (T units) =

INI PRE (P units) =

If thermo is different from global (GENeral section) options THEN select

K-value option

Enthalpy option

Density option

KKE =

HKE =

DKE =

Phase Map Examples

There are several sample flowsheets in "Chapter 34: Phase Map Samples - c:\designii\samples\equipment\phasemap" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 31: Plate-Fin Exchanger

The Plate-Fin Exchanger module can be used to simulate multiple stream exchangers. This type of exchanger allows multiple hot and cold streams to have heat exchange with maximum surface area. The module calculates the heat and material balance from known input stream information and the specification to be met.

Plate-Fin Exchanger Features

A typical plate-fin exchanger is composed of a "core" of alternating layers of shaped fins, providing flow channels with a large heat transfer area, and flat separator sheets, which separate these channels from each other.

Incoming streams are split between a number of the flow channels, in a configuration usually determined by the considerations of optimum heat transfer. Each stream may make a number of co- or counter-current passes through the core.

The module can be used in either of the two ways:

- without rating, to perform a thermodynamic calculation only. This is the general mode used to calculate the temperature change in the streams and provide enthalpy balances.
- with rating, to perform rigorous heat exchange and pressure drop calculations based on the geometry of the exchanger.

The optional Plate-Fin Exchanger Rating commands allow the rating of the brazed aluminum plate-fin exchangers found in gas processing industry. For example, it can be used to gauge the effect of changing the flow through the exchanger when the exchanger throughput may be a physical constraint on the process optimization.

Plate-Fin Exchanger Command Details

Required Specifications

NUMBER of HOT streams = Enter the number of hot side streams from the plate-fin exchanger.

Additional Commands

As Specifications

The following commands are used as specifications when rating is not performed. They will be met as per user specification.

As a starting guess

When RATING is done, these commands and data entered will be used as starting initial guesses. Converged temperatures are then obtained for the exit cold and hot side streams based on the plate-fin geometry commands. The default is **TEMPerature APPROach HOT stream** = 5.

TEMPerature OUT HOT stream (T units) = stream 1, stream 2,
Enter the estimate or specified temperature of the hot (gives up heat) outlet stream.

TEMPerature OUT COLD stream (T units) = stream 1, stream 2,
Enter the estimate or specified temperature of the cold (absorbs heat) outlet stream.

TEMPerature APPROach HOT side (T units) =
Enter temperature approach desired for cold side outlet stream.

TEMPerature APPROach COLD side (T units) =
Enter temperature approach desired for hot side outlet stream.

DUTy of hot side (Hunits/ t units) = stream 1, stream 2,
Enter the desired enthalpy change or duty available for the HOT side stream. This is the duty of each hot side stream of plate-fin exchanger. The overall duty will be the sum of these individual duties.

OUTlet STREAM PHAse = stream 1, stream2,
Sets the phase condition of the outlet streams. The phase condition is set for hot side stream outlets first and then cold side stream outlets. The four choices are from 1 - vapor, 2 - liquid, 3 - bubble point, 4 - dew point. Default is 0 - as calculated. NOTE: The use of this command will override all the above commands.

Plate - Fin Exchanger Optional Command Details

DELta pressure (P units) = stream 1, stream 2,
Enter the desired change in pressure across the heat exchanger for each of the hot and cold streams respectively.

EXChanger AREa (L2 units) = stream 1, stream 2,
Enter this command to specify the total heat exchanger area for each stream. By default, the area is calculated from the

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supplied geometry. If you enter this command the specified value will override the value calculated from the geometry.

Flow AREA (L2 units) = stream 1, stream 2,

Enter this command to specify the cross-sectional area through which each exchanger stream flows. By default, the area is calculated from the supplied geometry. It is normally not used.

Pressure OUT (P units) = stream 1, stream 2,

Enter the desired discharge pressure for each of the hot and cold streams respectively. Defaults to feed inlet pressure or frictional delta pressure if RATING is turned on.

Q-T

Enter this command to have duty versus temperature curves plotted for heat exchangers.

The Q-T table and plot are useful tools for evaluating exchanger design. These curves are based on end-point temperature results. You can quickly determine the minimum temperature approach or locate regions with unrealistically high $U \times A$ or temperature crossovers. In addition, bubble points and dew points are marked when vaporization or condensation occurs for either hot or cold streams.

Plate-Fin Exchanger Rating

The rating calculations are performed for plate-fin exchangers. DESIGN II first performs the calculation using the specifications you have entered to calculate outlet stream temperatures and total duty. All required properties for the rating calculation, such as viscosities, specific heats, thermal conductivities, densities, phase composition, and mass flows are automatically calculated for inlet and outlet conditions of both streams.

As with other required commands, values applying to streams are entered in the order that the stream numbers are listed in the primary module command with hot side being first, followed by cold side streams (eg. PFX 101=s1,s2,-s3,-s4). If only one value is given, it is assumed to be applicable to all streams.

Plate-Fin Exchanger: Calculation Commands

RATING on

You must enter this command to perform a rating calculation.

FOUling FACTor (1/U units) = stream 1, stream 2,

Enter the fouling factor for each stream. Default is 0.001 1/BTU/FT²/HR/ F. Other Units allowed are 1/KCAL/M²/HR/C, 1/KJ/M²/SEC/K, 1/CAL/M²/HR/C.

U-M = method

This is the calculation method employed for the calculation of overall heat transfer coefficient for each stream. TWO choices are available:

- 1 (default) uses the average difference between the wall and the fluid temperature. This is normally the most stable method.
- 2 uses an average cube root mean temperature difference between wall and fluid.

H-M = method

There are two methods to calculate the enthalpy changes occurring in the plate-fin exchanger.

- 1 (default) The first method uses an interpolation table to obtain node enthalpies.(choice = 1) This is the default method.
- 2 The second method uses flash calculations to determine node enthalpies (choice = 2).

UFActors = stream 1, stream 2,

Enter this command to adjust the Overall Heat Transfer Coefficient. It provides a "de-rating" factor for each stream which will be multiplied with the calculated heat transfer coefficient. The default is 1

NUMBER of **INC**rements = number

Enter this command to specify the number of segments into which the exchanger is to be divided for the rating calculation. The accuracy of the rating is increased by increasing the number of increments. However, the rating will take longer to run and convergence will be more difficult to achieve as the number of increments are increased. The default is 5.

INCrement **FRA**ctions =

Enter the cumulative length of the increments. The number of values is the number of increments plus one. The default is from zero to one using evenly spaced increments. For instance, if NUM INC = 5 then the default is "INC FRA = 0, 0.2, 0.4, 0.6, 0.8, 1".

TEMperature **PRO**file ith stream (T units) = node 1, node 2,

This command is used to provide initial temperature estimates at each node in the exchanger for the ith stream. The feed temperature is the first value entered. The values of the first and last entry will be overwritten by the exchanger inlet and outlet temperatures.

Plate-Fin Exchanger: Fin Commands

FIN TYPE = stream 1, stream 2

Enter this command to specify the fin type of the plate-fin exchanger.

Choices available are: 1 - Offset/serrated (lanced); 2 - Perforated, 3 - Plain (straight). Default is 1.

FIN HEIGHT (L units) = stream 1, stream 2

Enter this command to specify the fin height. The default is 0.28 inches.

FIN offset LENGTH (L units) = stream 1, stream 2

Enter this command to specify the fin length. This command is applicable when offset fins are used for stream passages. The default is 0.021 ft.

FIN THICKNESS (L units) = stream 1, stream 2

Enter this command to specify the thickness of fin metal. The default is 0.0013 ft (0.016 in). Typical heat transfer fin thickness range from 0.006 to 0.023 inches.

FIN PITCH (1/L units) = stream 1, stream 2

Enter this command to specify the fin spacing or number of fins per inch measured perpendicular to the direction of flow of each stream. The default is 17 fins per inch (204 fins per foot).

FIN PERFORATION (percent) = stream 1, stream 2

Enter this command to specify the fin perforation percent. The default is 5 percent.

FIN CONDUCTIVITY (H units/t units/L units/T units) =

Enter the average thermal conductivity of the fin material. Default is 100 BTU/HR/FT/F (English).

FIN FACTOR = stream 1, stream 2

Enter this command which provides a fractional factor for each stream which characterizes the fin efficiency (measure of effectiveness of the fin for heat transfer to the fluid channel) based on the exchanger stacking arrangement. Default is 1.

A method for determining these factors is itemized below:

- List the sequence of stream channels for the exchanger
- Consider each stream in turn and note the value for each channel occurrence for the stream.
- A value of 1.0 for a channel which is between two channels of the opposite type (i.e. a hot stream channel between two cold streams channels, or vice-versa)
- A value of 0.5 for a channel which is between a channel of the same type and one of the opposite type-for example, a hot stream channel which has a hot stream channel on one side and a cold stream channel on the other.
- A value of 0.0 for a channel which is between two channels of the same type, if this occurs.
- Total the value for the stream and divide by the number of values to obtain the average. This is the FIN FACTOR for that stream.

Plate-Fin Exchanger: Plate Commands

PLATE THICKNESS (L units) =

Enter this command to specify the parting sheet or plate thickness. The default is 0.08 inches.

PLATE CONDUCTIVITY (H units/t units/L units/T units) =

Enter the average thermal conductivity of the plate material. The default is 100 BTU/HR/FT/F (English).

Plate-Fin Exchanger: Configuration Commands

The configuration commands are used to describe the physical configuration of the Plate-Fin Exchanger (PFX).

EFFECTIVE passage LENGTH (L units) = stream 1, stream 2,

Specify the effective passage length along the direction of flow that each stream is in the effective heat exchange zone. Default is 120 inches (10 ft,) implying an exchanger 10 ft long.

EFFECTIVE passage WIDTH (L units) = stream 1, stream 2,

Specify the effective passage width perpendicular to the direction of flow that each stream is in the effective heat exchange zone. Default is 36 inches (3 ft), implying an exchanger 3 ft long.

NUMBER in PARALLEL =

Enter the number of plate-fin exchanger cores in parallel. The default is 1. When a value is entered, it is used for all streams.

NUMBER in SERIES =

Enter the number of plate-fin exchanger cores in series. The default is 1. When a value is entered, it is used for all streams.

NUMBER of LAYERS = stream 1, stream 2

Enter this command to specify the number of finned layers or flow passages per stream. The default value for each stream is 20, meaning that each stream flows through 20 inter-plate spaces for each pass through the exchanger.

Plate-Fin Exchanger Command Summary

Required Specifications

NUMBER of **HOT** streams =

Additional Commands

The following commands are NOT required but can be used. The default is **TEMP**erature **APPRO**ach **HOT** = 5.

TEMPerature **OUT HOT** of stream (T units) =
TEMPerature **OUT COLD** of stream (T units) =
TEMPerature **APPRO**ach **HOT** side (T units) =
TEMPerature **APPRO**ach **COLD** side (T units) =
DUTy of hot side (Hunits/ t units) =
OUTlet **ST**ream **PH**ase =

Optional Commands

DELta pressure (P units) =
EXchanger **ARE**a (L2 units) =
FLOW AREa (L2 units) =
PREssure **OUT** (P units) =
Q-T

Plate-Fin Exchanger Rating Commands

RATING
U-M =
H-M =
NUMBER of **LAY**ers =
NUMBER of **INC**rements =
INCrement **FRA**ctions =
TEMPerature **PRO**file ith stream (T units) =
FIN TYPE =
FIN HEIght (L units) =
FIN offset **LENG**th (L units) =
FIN THickness (L units) =
FIN PERforation (percent) =
FIN PITCH (1/L units) =
FIN CONductivity (H units/t units/L units/T units) =
FIN FACTor =
UFActors =
FOULing **FACT**or =
EFFective passage **LENG**th (L units) =
EFFective passage **WID**th (L units) =
NUMBER in **PAR**allel =
NUMBER in **SER**ies =
PLAte **TH**ickness (L units) =
PLAte **CON**ductivity (H units/t units/L units/T units) =

Thermodynamic Commands

HKEy =
KKEy =
DKEy =

Plate-Fin Exchanger Step by Step

Plate-Fin Exchanger STEP 1

Enter all the information at the right to uniquely define the module and its connections to the rest of the flowsheet. Equipment name and connectivity (ALL are required).

Equipment module identifier

PFX

Equipment number

Assigned equipment flowsheet number

Equipment name	User choice - up to 16 characters
Inlet stream(s)	Up to 10 streams
Outlet stream(s)	Up to 10 streams.

Plate-Fin Exchanger STEP 2

Enter the module description. Required module description (enter the FIRST of the following). The following additional commands are used as specifications when rating is not performed. They will be met as per user specifications.

When RATING is done, these additional commands and data entered will not be used as starting initial guesses. Converged temperatures are then obtained for the exit cold and hot side streams based on the plate-fin geometry commands. The default is TEMperature APProach HOT stream = 5.

The module can be used in either of the two ways:

- without rating, to perform a thermodynamic calculation only. This is the general mode used to calculate the temperature change in the streams and provide enthalpy balances.
- with rating (after completing commands below include Plate-Fin Exchanger Step 3), to perform rigorous heat exchange and pressure drop calculations based on the geometry of the exchanger.

Required Specifications

Enter the number of hot side streams for the plate-fin exchanger.

NUM HOT =

Additional Commands

Enter the estimate or specified temperature of the hot (gives up heat) outlet stream

TEM OUT HOT (T units)
=s1,s2

Enter the estimate or specified temperature of the cold (absorbs heat) outlet stream.

TEM OUT COLD (T units)
=s1,s2

Enter temperature approach desired for cold side outlet stream.

TEM APP HOT (T units) =

Enter Temperature approach desired for hot side outlet stream.

TEM APP COLD (T units) =

Enter the desired enthalpy change or duty available for the HOT side stream. This is the duty of each hot side stream of the plate-fin exchanger.

DUTy (H units/ t units) =s1,s2

Sets the phase condition of the outlet streams. The phase condition is set for hot side stream outlets first, and then cold side stream outlets. The four choices are from 1- vapor, 2- liquid, 3 – bubble point, 4 – dew point. Default is 0 – as calculated. NOTE: The use of this command will override all the above commands.

OUT STR PHA = s1, s2

Optional Commands

Enter the desired change in pressure across the heat exchanger for each of the hot and cold streams respectively.

DEL (P units) = s1,s2

Enter this command to specify the total heat exchanger area for each stream. By default, the area is calculated from the supplied geometry. If you enter this command the specified value will override the value calculated from the geometry.

EXC ARE (L2 units) = s1,s2

Enter this command to specify the cross-sectional area through which each exchanger stream flows. By default, the area is calculated from the supplied geometry. It is normally not used.

FLO ARE (L2 units) = s1,s2

Sets the phase condition of the outlet streams. The four choices are from 1 - vapor, 2 - liquid, 3 - bubble point, 4 - dew point.

OUT STR PHA = s1, s2

Enter the desired discharge pressure for each of the hot and cold streams respectively. Defaults to feed inlet pressure or frictional delta pressure if RATING is turned on.

PRE OUT (P units) = s1, s2

Enter this command to have duty versus temperature curves plotted for heat exchangers.

Q-T

The Q-T table and plot are useful tools for evaluating exchanger design.

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These curves are based on end-point temperature results. You can quickly determine the minimum temperature approach or locate regions with unrealistically high $U \times A$ or temperature crossovers. In addition, bubble points and dew points are marked when vaporization or condensation occurs for either hot or cold streams

Plate-Fin Exchanger STEP 3

Enter the required specifications and options for plate-fin exchanger rating.

Plate-Fin Exchanger rating options (enter the following required command).

Plate-Fin Exchanger Rating ON

RAT

Configuration Commands

Specify the effective passage length along the direction of flow that each stream is in the effective heat exchange zone. Default is 120 inches (10 ft.), implying an exchanger 10 ft long.

EFF LEN (L units) = s1, s2

Specify the effective passage width perpendicular to the direction of flow that each stream is in the effective heat exchange zone. Default is 36 inches (3 ft.), implying an exchanger 3 ft long.

EFF WID (L units) = s1, s2

Enter the number of plate-fin exchangers in parallel. The default is 1. When a value is entered, it is used for all streams.

NUM PAR = number

Enter the number of plate-fin exchangers in series. The default is 1. When a value is entered, it is used for all streams.

NUM SER =

Enter this command to specify the number of finned layers or flow passages per stream. The default value for each stream is 20, meaning that each stream flows through 20 inter-plate spaces for each pass through the exchanger.

NUM LAYERS = s1, s2

Calculation Commands

Enter the fouling factor for each stream. Default is 0.001 hr-ft²-F/btu.

FOU FAC (1/U units) = s1, s2

This is the calculation method employed for the calculation of overall heat transfer coefficient for each stream. Two choices are available:

U-M = method,

1. (default) uses the average difference between the wall and the fluid temperature. This is normally the most stable method.
2. uses an average cube root mean temperature difference between wall and fluid.

There are two methods to calculate the enthalpy changes occurring in the plate-fin exchanger.

H-M = method

1. The first method uses an interpolation table to obtain node enthalpies.(choice = 1) This is the default method.
2. The second method uses flash calculations to determine node enthalpies (choice = 2).

Enter this command to adjust the Overall Heat Transfer Coefficient. It provides fractional "de-rating" factor for each stream which will be multiplied with the calculated heat transfer coefficient. The default is 1.

UFA = s1, s2,

Enter this command to specify the number of segments into which the exchanger is to be divided for the rating calculation. The accuracy of the rating is increased by increasing the number of increments. However, the rating will take longer to run and convergence will be more difficult to achieve as the number of increments are increased. The default is 5.

NUM INC =

Enter the cumulative length of the increments. The number of values is the number of increments plus one. The default is from zero to one using evenly spaced increments. For instance, if NUM INC = 5, then the default is "INC

INC FRA =

FRA = 0, 0.2, 0.4, 0.6, 0.8, 1"

This command is used to provide initial temperature estimates at each node in the exchanger. Do not specify the feed temperature for the ith stream. The feed temperature is the first value entered. The values of the first and last entry will be overwritten by the exchanger inlet and outlet temperatures.

TEM PRO ith stream (T units)
= node 1, node 2

Fin Commands

Enter this command to specify the fin type of the plate-fin exchanger. Choices available are: 1 – Offset/serrated (lanced); 2 - Perforated, 3 - Plain (straight). Default is 1.

FIN TYP =s1, s2

Enter this command to specify the fin height. The default is 0.28 inches

FIN HEI (L units) = s1, s2

Enter this command to specify the fin length. This command is applicable when offset fins are used for stream passages. The default is 0.25 inches.

FIN LEN (L units) = s1,s2

Enter this command to specify the thickness of fin metal. The default is 0.0013 ft (0.016 in). Typical heat transfer fin thickness range from 0.006 to 0.023 inches.

FIN THI (L units) = s1, s2

Enter this command to specify the the fin spacing or number of fins per inch measured perpendicular to the direction of flow of each stream. The default is 17 fins per inch (204 per foot).

FIN PIT (1/L units) = s1, s2

Enter this command to specify the fin perforation percent. The default is 5 percent.

FIN PER (percent) = s1, s2

Enter the average thermal conductivity of the fin material. Default is 100 BTU/HR/FT/F (English).

FIN CON (H units/t units/L units/T units) =

Enter this command which provides a fractional factor for each stream which characterizes the fin efficiency (measure of effectiveness of the fin for heat transfer to the fluid channel) based on the exchanger stacking arrangement. Default is 1.

FIN FAC = s1, s2

Plate Commands

Enter this command to specify the parting sheet or plate thickness. The default is 0.08 inches.

PLA THI (L units) =s1, s2

Enter the average thermal conductivity of the plate material. The default is 100 BTU/HR/FT/F (English).

PLA CON (H units/t units/L units/T units) =

Plate-Fin Exchanger Examples

There are several sample flowsheets in "Chapter 34: Phase Map Samples - c:\designii\samples\equipmnt\phasemap" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 32: Plug Flow Reactor

The PLUG FLOW REACTOR (PFR) module calculates single-phase reactions using specified information on the reactor dimensions, stoichiometric coefficients of the reactants and products, and power law rate expressions. Alternate methods for specifying reaction kinetics are available in the form of keyword commands or using Inline FORTRAN. Heat of formation data is required for any component with an ID number greater than 98. Enter this data in the GENERAL section of the input file via the HEAT of FORMation command.

When the plug flow reactor module is used, only a single stream for the reactor feed may be coded. If a cooling stream is required, it must be coded as the second inlet stream. Limiting assumptions by the module include no radial mixing, concentrations of reacting species vary only along the length of the reactor, and except for isothermal operation, the temperature varies along the length of the reactor. Default values will be used where indicated if no value is entered by the user.

Plug Flow Reactor Types

The four types of PFR which can be modeled are

- Isothermal
- Temperature profile
- Adiabatic
- Cocurrent coolant

Results

PFR results will be reported in the "NOW CALLING" section of the output file (mass basis) and compositions for the product stream will be in the Stream Summary and Detailed Stream Report. Reactions and overall duty for the reactor will be reported in the Equipment Summary.

Method of Calculation

The default rate expressions are the power law type with the rate constant expressed by the Arrhenius equation

$$k = k_o e^{E_o/RT}$$

where k_o is the frequency factor, E_o is the activation energy, R is the molar gas constant and T is the temperature.

Alternatively, rate expressions can be entered with Inline FORTRAN statements using the DURING option. The reactions are integrated along the length of the reactor using the Gear integration method.

Plug Flow Reactor Command Details

Plug Flow Reactor: Major Specifications

(enter both of the following)

DIAMeter (L units) =

Enter the internal diameter of the reactor.

LENGth (L units) =

Enter the length of the reactor.

Plug Flow Reactor: Type Specification

TYPE =

Reactor type keyword command. Reactor type options are shown below.

(choose only one of the following)

ISOthermal

Product stream enthalpy is calculated using the feed stream temperature. No additional commands are required for this reactor.

TEMperature **PRO**file

Allows the input of a temperature profile (required) along the length of the reactor.

ADIabatic

Product stream enthalpy is equal to the feed stream enthalpy plus the heat of reaction, and the temperature of reactor product is calculated. Also allows an optional heat duty specification which is transferred equally along the reactor length.

COCurrent

Allows the input of a cooling stream and the specification of an overall heat transfer coefficient between the cooling stream and the reactants. To use this reactor type, a second inlet stream must be coded.

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Plug Flow Reactor: Temperature Profile Commands

(following command is required)

TEMPerature **PRO**file (T units) = p1 ,T1 , ...,pn ,Tn

Enter the temperature profile where "p" is the relative position from the entrance of the reactor on a fractional basis and "T" is the temperature at position "p" . The program will interpolate temperature linearly from your profile.

Plug Flow Reactor: Adiabatic Reactor Commands

(command is optional)

HEAt added (H units/t units) =

Enter an optional heat duty specification to be transferred equally along the reactor length.

Plug Flow Reactor: Cocurrent Reactor Specifications

(choose any of the following commands)

COOLant **STReam** = i

Enter a stream number for "i" to be used as a coolant stream. The second inlet stream will be used automatically as the coolant stream unless specified otherwise.

COOLant **PRE**ssure **DRO**p (P units) =

Enter a pressure drop for the coolant stream.

TEMPerature **APPR**oach (T units) =

Enter a minimum approach temperature between the reactants and coolant streams. The calculation will not be interrupted if the temperature approach falls below the minimum, however, the program will print a warning message. Default is 5F.

U (U units) =

Enter the overall heat transfer coefficient between the coolant stream and the reactor. Default is 50 BTU/HR-FT²-F.

Plug Flow Reactor: Reaction Stoichiometry Commands

R i = (a1*r1+ a2*r2 + = b1*p1 + b2*p2 +

Enter a reaction command for each reaction.

where:

i	is the reaction number
a1,a2	are stoichiometric coefficients for the reactants
r1,r2	are component ID numbers for the reactants
b1,b2	are stoichiometric coefficients for the products
p1,p2	are component ID numbers for the products.

NOTE: Up to **24 reactions** are allowed per plug flow reactor module.

Plug Flow Reactor: Reaction Kinetics Commands

All of the following commands are required, regardless of the reactor type you have chosen. These three items, which determine the rate of the reaction, can also be defined using Inline FORTRAN. This allows you to override the power law model by specifying the kinetics directly.

ORDer of reaction **i** = r1, Or1, r2, Or2

Enter the partial order of each reactant

where:

i	is the reaction number,
r1,r2	are component ID numbers for the reactants,
Or1,Or2	are partial orders for the corresponding reactant.

FREquency factor (L3 units,molar Q units,t units) =

i1, fi1, i2, fi2 Enter the frequency factor (ko)

where: i1, i2 are the reaction numbers
fi1, fi2 are the frequency factors for the corresponding reaction.

NOTE: The order of the dimensional units for the FREquency factor command cannot be changed. The program will automatically determine whether volume or area units are appropriate from the ORDer command.

ACTivation energy (H units/molar Q units) =

i1, Ei1, i2, Ei2 Enter the activation energy (Eo)

where: i_1, i_2 are the reaction numbers
 E_{i1}, E_{i2} are the activation energies for the corresponding reaction.

RATE $i = f(\text{CONC}_j, \text{TEM}, \text{PRE})$

The FRE, ORD, and ACT commands can be replaced with an Inline FORTRAN expression called DURING.

where: i is the reaction number,
 RATE is a required Inline FORTRAN keyword,
 CONC is a keyword representing concentration,
 Default units: LBMOL/FT³
 j is the component ID number,
 TEM is a keyword for temperature within the reactor,
 Default units: degree Rankine
 PRE is a keyword for pressure within the reactor.
 Default units: PSIA

Example using Inline FORTRAN to replace FRE, ORD, and ACT commands

```
Component ID:      22      1      3
Reaction:          C2 H4+ H 2 ----->> C2 H6
                  ko = 5.0457 E13 FT2/LBMOL-HR
                  Eo= 5.8845 E4 BTU/LBMOL
```

The rate of this reaction can be expressed as frequency

$$e = \frac{E_o}{R \cdot \text{TEM}} \cdot \text{CONC}_y \cdot \text{CONC}_x$$

where:

R is the gas constant,
 y is the power term for ethylene,
 x is the power term for hydrogen.

Using Inline FORTRAN, the coding for reaction rate is expressed as:

```
R2 = (1*22 + 1*1 = 1*3)
F-   DURING
F-   RATE2 = 5.0457E13*EXP(-.58845E4/(R*TEM)) *CONC22*CONC1
```

Plug Flow Reactor: Required Commands For Components With Id Numbers > 99

The DESIGN II database contains heat of formation data for components with ID numbers from 1 through 99. If you specify a component with an ID greater than 98, you must supply its corresponding heat of formation data. Enter heat of formation data with one of the following commands depending on the basis of the available data (vapor or liquid). The selected command must appear in the GENeral section.

HEAT of FORMation (H units/molar Q units) $i =$

Enter the heat of formation for component "i", where "i" is the component ID number. Use when data is on a vapor basis.

HEAT of FORMation of LIQuid (H units/molar Q units) $i =$

Enter the heat of formation for component "i", where "i" is the component ID number. Use when data is on a liquid basis.

NOTE: Air (component 99) should not be used in reaction calculations where oxygen or nitrogen species would be reacting. Define the air stream using O₂ (component 47) and N₂ (component 46)

For example,

```
GENeral
COMPonents = 2,49,48,62,1021
HEAT of FORMation (BTU/LBMOL) 1021 = -86544
```

Plug Flow Reactor Optional Command Details

(Choose any of the following commands)

NUMBER of INCrements =

Compositions, temperature, and pressure will be shown for the reactor inlet, outlet, and several intermediate points. Default for increments is 10.

DELta pressure (P units) =

Enter a pressure drop for the reactor.

Lost Work Analysis

If a lost work analysis is specified with the LOST work command in the GENeral section, the ENTropy of FORmation data must also be entered in the GENeral section with the following command.

ENTropy of **FOR**mation (H units/molar Q units/T units) **i** =

Enter the entropy of formation data for any components with id numbers greater than 99. Default is 0.0.

Allowable entropy units are:

BTU/LBMOL/R (default)
J/GMOL/K

CAL/GMOL/K
KCAL/KGMOL/K

KJ/KGMOL/K

Plug Flow Reactor Command Summary

Major Specifications

DIAmeter (L units) =

LENgth (L units) =

Reactor Type Specifications

TYPE =

ISOthermal

TEMperature **PRO**file

ADIabatic

COCurrent

Temperature Profile Reactor Commands

TEMperature **PRO**file (T units) = $p_1 T_1, \dots, p_n, T_n$

Adiabatic Reactor Commands

HEAt added (H units/t units) =

Cocurrent Reactor Specifications

COOlant **ST**ream = **i**

COOlant **PRE**ssure **DRO**p (P units) =

TEMperature **APP**roach (T units) =

U (U units) =

Reaction Stoichiometry Commands

R i = ($a_1^* r_1 + a_2^* r_2 + \dots = b_1^* p_1 + b_2^* p_2 + \dots$)

Reaction Kinetics Commands

ORder of reaction **i** = $r_1, Or_1, r_2, Or_2 \dots$

FREquency factor (L³ units, molar Q units, t units) = $i_1, f_{i1}, i_2, f_{i2} \dots$

ACTivation energy (H units/molar Q units) = $i_1, E_{i1}, i_2, E_{i2} \dots$

or

RATe **i** = $f(\text{CONC}_i, \text{TEM}, \text{PRE})$

Optional Commands

NUMber of **INC**rements =

DELta pressure (P units) =

Additional Component Specification Commands

HEAt of **FOR**mation (H units/molar Q units) **i** =

HEAt of **FOR**mation of **LIQ**uid (H units/molar Q units) **i**

=

ENTropy of **FOR**mation (H units/molar Q units/T units) **i**

=

Thermodynamics Commands

HKEy =

KKEy =

DKEy =

Plug Flow Reactor Step by Step

Plug Flow Reactor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

PLU REA

Assigned equipment flowsheet number

User choice - up to 16 characters

One or two, If two 1st is feed, 2nd is coolant

Specify one; two if COCurrent reactor used

Plug Flow Reactor STEP 2

Specify the diameter and length of the reactor. Reactor dimensions specification (enter BOTH of the following commands)

Diameter

Length

DIA (L units) =

LEN (L units) =

Plug Flow Reactor STEP 3

Choose one of the four reactor types listed below. Isothermal reactor (enter the following command)

Isothermal reactor keyword command

TYP = ISO

Temperature profile reactor (enter BOTH of the following commands)

Temperature profile reactor keyword command

Temperature profile specification

TYP = TEM PRO

TEM PRO (T units) = $p_1, T_1, \dots, p_n, T_n$

- pi position relative to the reactor entrance on a fractional basis
- Ti temperature at position pi

Adiabatic reactor (enter BOTH of the following two commands)

Adiabatic reactor

Optional heat duty specification (transferred equally along the reactor length)

TYP = ADI

HEA (H units/t units) =

Cocurrent reactor (enter following commands)

Cocurrent reactor

Optional cooling stream specification (second inlet stream will be used as the coolant stream unless specified otherwise)

Optional pressure drop specification for the coolant stream

Optional minimum temperature approach specification (a warning message is printed if the temperature approach falls below this approach; default is 5 F)

Optional overall heat transfer coefficient specification between the coolant stream and the reactor (default is 50 BTU/HR-FT²-F)

TYP = COC

COO STR = i

COO PRE DRO (P units) =

TEM APP (T units) =

U (U units) =

Plug Flow Reactor STEP 4

Enter the information required listed below to define reaction stoichiometry.

Reaction stoichiometry for each reaction

R i = (a1*r1 + a2*r2 + .. = b1*p1 + b2*p2 + ..)

- i reaction number
- a1,a2 stoichiometric coefficients for the reactants
- r1,r2 component ID numbers for the reactants
- b1,b2 stoichiometric coefficients for the products
- p1,p2 component ID numbers for the products

Plug Flow Reactor STEP 5

Enter the information listed below to define the reaction kinetics (power law) or use Inline FORTRAN to define reaction kinetics. Partial order of each reactant.

Order of reaction

ORD i = r1, Or1, r2, Or2

- i reaction number
- r1,r2 component ID numbers for the reactants
- Or1,Or2 partial orders for the corresponding reactant

Frequency factor (ko) and activation energy Eo) specification

Frequency factor (order of the dimensional units for the FREquency factor command cannot be changed)

FRE (L3 units, molar Q units, t units) = i1,fi1,i2,fi2 ..

- i 1,i2 reaction numbers
- fi1,fi2 frequency factors for the corresponding reaction

Activation energy

ACT (H units/molar Q units) = i1,Ei1,i2,Ei2 ..

- i1,i2 reaction numbers
- Ei1,Ei2 activation energies for the corresponding reaction

Inline FORTRAN reaction kinetics command

Rate (see reference section for additional information)

RAT i = F (CONCj, TEM, PRE)

- i reaction number
- RAT required inline FORTRAN keyword
- CONC keyword representing concentration
- j component ID number
- TEM keyword for temperature within the reactor
- PRE keyword for pressure within the reactor

Plug Flow Reactor STEP 6

Enter heat of formation data for components with ID numbers > 98

Enter ONE of the following heat of formation commands based on the reactor feed phase.

- Heat of formation of component "i", where "i" is the component ID number. Used when data is on a vapor basis (place command in the GENeral section) **HEA FOR** (H units/molar Q units) i =
- Heat of formation of component "i", where "i" is the component ID number. Used when data is on a liquid basis (place command in the GENeral section) **HEA FOR LIQ** (H units/molar Q units) i =

OPTIONAL - Choose any of the optional commands listed below:

Chapter 32

Number of equally spaced points to display compositions,
temperature and pressure along the reactor (default is 10)
Pressure drop for the reactor

NUM INC =

DEL (P units) =

If LOST work command is entered in GENeral section, THEN enter the following:

Entropy of formation where "I" is the component ID number. (Enter
this command in the GENeral section)

ENT FOR (H units/molar Q units/T units) i =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Plug Flow Reactor Examples

There are several sample flowsheets in "Chapter 36: Plug Flow Reactor Samples - c:\designii\samples\equipmnt\plugreac" of the DESIGN II for Windows Tutorial and Samples Guide.

Plug Flow References

1. Smith, J.M., *Chemical Engineering Kinetics*, 3rd Ed., M1981.
2. Froment, Gilbert F., and Bischoff, Kenneth B., *Chemical Reactor Analysis and Design*, John Wiley & Sons, New York, 1979.

Chapter 33: Polytropic Compressor

(Centrifugal Compressor and Pump)

The POLytropic compressor module is used to simulate a single stage of a centrifugal compressor based on manufacturer's performance curves. When it is used in conjunction with other DESIGN II modules, it is possible to simulate multistage compression with intercooling, recycle or kickback between stages, and to evaluate existing compressors under off-design conditions. For multistage compression, a separate POLytropic compressor module is used to simulate each stage. Each stage can have several wheels. HEAt EXChanger, FLAsh, and other modules can be added between stages for intercooling and liquid dropout effects. The polytropic efficiency and polytropic head (work/mass/rotational speed) must be provided as a function of capacity (inlet volumetric flowrate/rotational speed). If manufacturer's data is in a different form, the data can be recalculated and plotted into the required form. The POLy module calculates the outlet temperature and pressure, and the work consumed for a given suction stream and desired impeller speed. The speed can also be varied by the CONTroller module to achieve a desired outlet condition (e.g. pressure or temperature). Interpolation at the actual speed point will be performed when a specific speed point is entered between multiple speed points. The POLy module can also be used for modeling centrifugal pumps (the inlet stream should be all liquid) based on manufacturer's curves.

Polytropic Compressor Command Details

POLytropic EFFiciency in percent (L3/ t /R units or L3/t units) =

Enter up to 30 pairs of polytropic efficiency in percent versus capacity (actual volume flowrate/speed) points.

POLytropic HEAd (H/mass Q/R2 units or H/mass Q units, L3/ t /R units or L3/t units) =

Enter up to 30 pairs of polytropic head versus capacity points.

SPEed of impeller (R units) =

Enter the rotational velocity of the impeller.

For **Multiple Speed Curves** following commands apply:

POLytropic EFFiciency in percent (L3/ t /R units or L3/t units) speed =

Enter up to 30 pairs of polytropic efficiency in percent versus capacity (actual volume flowrate/speed) points.

POLytropic HEAd (H/mass Q/R2 units or H/mass Q units, L3/ t /R units or L3/t units) speed =

Enter up to 30 pairs of polytropic head versus capacity points.

NOTE: Interpolation at the actual speed point will be performed when a specific speed point is entered between multiple speed points. Up to ten vendor performance speed curves can be entered.

Polytropic Compressor Optional Command Details

PREssure OUT (P units) =

Enter guess for discharge pressure. Default is 2.5 times the inlet pressure.

THERmodynamic FACTor =

Enter a factor (usually between 0.9 and 1.1) to correct the manufacturer's curves for the thermodynamic option you select. Default is 1.0.

TOLerance =

Enter the relative tolerance for convergence. Default is 0.001.

Polytropic Compressor Command Summary

Required Commands

POLytropic EFFiciency in percent (L3/t/R units or L3/t units)
= *data pairs*

POLytropic HEAd (H/mass Q/R2 units or H/mass Q units,
L3/t/R units or L3/t units) = *data pairs*

SPEed of impeller (R units) =

Multiple Speed Curve Commands

POLytropic EFFiciency in percent (L3/t/R units or L3/t units)
speed = *data pairs*

POLytropic HEAd (H/mass Q/R2 units or H/mass Q units, L3/t/R
units or L3/t units) speed = *data pairs*

Optional Commands

PREssure OUT (P units) =

THERmodynamic FACTor =

TOLerance =

HKEy =

KKEy =

DKEy =

Polytropic Compressor Step by Step

Polytropic Compressor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier	POL
Equipment number	Assigned equipment flowsheet number
Equipment name	User choice - up to 16 characters
Inlet stream	Unlimited in number
Outlet streams	Specify only one

Polytropic Compressor STEP 2

Enter the rotational velocity of the impeller.

Speed of impeller	SPE (R units) =
-------------------	------------------------

Polytropic Compressor STEP 3

Enter polytropic efficiency and head versus capacity points.

Polytropic efficiency in percent versus capacity	POL EFF in percent (L3/t/R units or L3/t units) =
Polytropic head versus capacity	POL HEA (H/mass Q/R2 units or H/mass Q units, L3/t/R units or L3/t units) =

Enter multiple speed curve points.

Polytropic efficiency in percent versus capacity	POL EFF in percent (L3/t/R units or L3/t units) speed =
Polytropic head versus capacity	POL HEA (H/mass Q/R2 units or H/mass Q units, L3/t/R units or L3/t units) speed =

OPTIONAL - Choose any of the optional specifications listed below. Pressure out, thermodynamic correction factor and tolerance

Pressure out guess (default is 2.5 times the inlet pressure)	PRE OUT (P units) =
Thermodynamic correction factor (default is 1.0)	THE FAC =
Relative convergence tolerance (default is 0.001)	TOL =

IF thermo is different from global (GENeral section) options THEN select

K-value option	KKE =
Enthalpy option	HKE =
Density option	DKE =

Polytropic Compressor Examples

There are several sample flowsheets in "Chapter 37: Polytropic Compressor Samples - c:\designii\samples\equipment\polycomp" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 34: Pump

The PUMp module pumps a liquid to a specified outlet pressure or to a pressure limited by a specified work available. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure. Only one output stream should be coded.

When vapor is found in the suction of the pump, a warning message is printed. If the ENTropy calculation is specified, a rigorous mixed-phase calculation is performed. If the ENTropy calculation is not specified, the vapor is pumped as if it were a liquid. If the **vapor fraction of the feed is greater than 0.5**, the calculation switches to the compressor option and a significant rise in calculated temperature may occur.

Pump Command Details

Pump Major Specifications

WORK AVAilable (p units) =

Enter the available work capacity. Default is 1 X 10E6 HP (7.457 X 10E8 WA).

The WORK AVAilable may limit the discharge pressure. Therefore, to achieve a desired work, be sure the PREssure OUT you specify is greater than can be obtained with specified WORK AVAilable.

PREssure OUT (P units) =

Enter the desired discharge pressure. When it is not specified, default is twice the suction pressure.

PREssure DELta (P units) =

Enter desired pressure change or delta pressure. When it is not specified, default is twice the suction pressure..

PREssure OUT is **DEW** point

and

TEMperature of DEW point (T units) =

The dew point pressure at the specified temperature is calculated and then used as the discharge pressure for the pump calculation. **Both commands must be used.**

PREssure OUT is **BUBble** point

and

TEMperature of BUBble point (T units) =

The bubble point pressure at the specified temperature is calculated and then used as the discharge pressure for the pump calculation. **Both commands must be used.**

NOTE: The discharge temperature is calculated by pumping the inlet stream to the bubble or dew point pressure and will not be the specified bubble or dew point temperature.

Pump Efficiency Commands

Choose only one of the THREE options; default is a volumetric efficiency of 0.9.

To simulate a centrifugal pump, you normally enter the efficiency using the following commands:

ENTropy calculation

and

EFFiciency = fraction

Enter the efficiency (from constant entropy). The default is 0.65. **Both commands must be used.**

The work is calculated from the enthalpy change resulting from a constant entropy pressure increase, divided by the efficiency.

To simulate a reciprocating pump, you normally enter the volumetric efficiency by specifying:

EFFiciency = **fraction**

If the ENTropy calculation is not specified, use this command to set the pump volumetric efficiency. The default value used is 0.90.

Remember that the volumetric efficiency does not take into account the mechanical efficiency, which must be applied by hand calculation.

To simulate a centrifugal pump, you can also enter the temperature out and the efficiency will be automatically calculated using the following command:

TEMperature OUT (T units) =

Enter desired temperature. Efficiency will be calculated.

Pump Optional Command Details

Driver Commands

The program always calculates the kilowatts required for electric motor drive (assuming 100 percent efficiency for the motor) or the fuel gas consumption, assuming a 980 BTU/SCF fuel (8.639 x 10⁵ KJ/KGMOL) and 8000 BTU/HR/HP (3.14 x 10⁻³ KJ/SEC/WA). The calculated value is printed in the equipment summary.

Electric drive is the default option for a non-entropy machine; fuel gas is the default option for an entropy machine. You can specify which option you want by using one of the two following commands:

Electric drive

FUEL gas

If you want the steam required for a steam drive to be calculated and reported in the equipment summary, enter both of the following commands.

STEam enthalpy **I**N (H/molar Q units) =

Enter the enthalpy of the steam at inlet to the driver.

STEam enthalpy **O**UT (H/molar Q units) =

Enter the enthalpy of the steam at exit from the driver.

Pump Command Summary

Major Specifications

WORk **A**VAilable (p units) =

PREssure **O**UT (P units) =

PREssure **D**ELta (P units) =

PREssure **O**UT is **D**EW point
and

TEMperature of **D**EW point (T units) =

PREssure **O**UT is **B**UBble point
and

TEMperature of **B**UBble point (T units) =

Efficiency Commands

ENTropy calculation
and

EFFiciency = *fraction*

EFFiciency = *fraction*

TEMperature **O**UT (T units) =
(Efficiency will be calculated)

Driver Commands

Electric drive

FUEL gas

STEam enthalpy **I**N (H/molar Q units) =

STEam enthalpy **O**UT (H/molar Q units) =

Thermodynamic Commands

HKEy =

KKEy =

DKEy =

Pump Step by Step

Pump STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

PUM

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

Specify only one

Pump STEP 2

Choose available work capacity or outlet pressure specification. Enter ONE of the following:

IF available work capacity (default is 10⁶ HP)

IF outlet pressure (select ONE of the following three options)

- Discharge pressure

- Pressure change or delta pressure

- Dew point pressure at temperature

WOR **A**VA (p units) =

PRE **O**UT (P units) =

PREssure **D**ELta (P units) =

PRE **O**UT **D**EW

- Bubble point pressure at temperature

TEM DEW (T units) =

PRE OUT BUB

TEM BUB (T units) =

Pump STEP 3

Choose the desired efficiency option. Default option is volumetric efficiency. Enter ONE of the following:

Entropy - Adiabatic efficiency (default is 0.65)

ENT, EFF = fraction

Temperature Out (*Efficiency will be calculated*)

TEM OUT (T units) =

OPTIONAL - Choose any of the optional specifications listed below. IF driver options THEN select ONE of the following driver options

Electric motor (default)

ELE DRI

Fuel gas turbine

FUEL

IF steam is required for your driver, THEN select BOTH of the following

Steam enthalpy in

STE IN (H/molar Q units) =

Steam enthalpy out

STE OUT (H/molar Q units) =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Pump Examples

There are several sample flowsheets in "Chapter 38: Pump Samples - c:\designii\samples\equipmnt\pump" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 35: Reactor

The REActor module calculates component distribution for the conditions existing at equilibrium, the heat released or absorbed during the reaction, and the resultant temperature changes. The temperature and enthalpy of the product are calculated based on the type of reactor.

For reactors with more than one reaction, the REActor module can be connected in series and each reaction simulated by a different REActor module. For a stoichiometric reaction, a vapor and a liquid product stream can be coded. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure before the reactor calculation is performed.

The calculation can only be performed if the resultant feed is totally vapor. A stoichiometric reaction, however, may have a two phase inlet stream. The equilibrium reactions are gas-phase reactions so equation of state options such as APISOAVE, SOAVE, REDLICH-KWONG, or PENG-ROBINSON should be used to model the thermodynamics.

NOTE: If the temperature out of the REActor will be in excess of 1000F, you should consider using VAPor PREssure K-values and IDEALH enthalpies or entering tabular K-values and enthalpies via a CHEmtran File.

Reactor Methodology

Method of Calculation

In all of the equilibrium reactors, the constituents of the reaction (such as CO, CO₂, H₂O, and H₂) are assumed to be in equilibrium at a certain temperature or varying degrees of approach to that temperature. The calculation proceeds until both heat and mass balance are achieved for a reaction or set of reactions. Feed compositions and flowrates can be entered for which no solution exist. In this case the program calculations will stop with a warning message. Calculations will also stop if the reactor feed(s) for the specific reaction types is not all vapor.

For the stoichiometric reactor, the calculations will proceed until the conversion of the limiting reactant is reached, or the limiting reactant is totally consumed. If a heat of reaction has been supplied, the value is multiplied by the moles of limiting reactant converted and the resulting enthalpy will be added to the feed enthalpy. The outlet temperature will be calculated based on the feed enthalpy and the product composition. For reactors which are defined as isothermal or specified outlet temperature, a reactor duty will be calculated.

NOTE: The simple (stoichiometric) reactor is like a black-box calculation. You can define reactions or conditions which are not physically or thermodynamically possible.

Reactor Command Details

Reactor: Types

(select only one)

ADiabatic reactor

Enter command keyword. Product stream enthalpy is equal to the feed stream enthalpy plus the heat of reaction, and the temperature of reactor product is calculated from the product composition and enthalpy. This is the default type.

ISOthermal reactor

Enter command keyword. For the ISOthermal reactor, the temperature of the feed is used as the temperature of the product.

The enthalpy of the product is calculated from product composition and feed temperature. For a simple reactor, the HEAT of reaction per mole of the limiting reactant can be specified. An enthalpy balance is then used to calculate the heat added or removed from the reactor to maintain constant temperature.

TEMperature OUT (T units) =

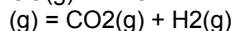
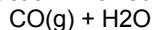
Enter the reactor product temperature. For the TEMperature OUT reactor, the specified product temperature is used with the product composition in calculating the product enthalpy. An enthalpy balance will be performed to calculate the amount of heat added to or removed from the reactor to meet the desired temperature.

Reactor: Specific Reaction Type Commands

(select only one)

COSHIFt reaction

The reaction involved is:

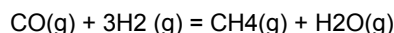
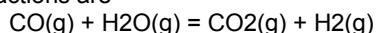


Methane, as well as other hydrocarbon components, will be treated as inert and will not affect the calculation. Oxygen cannot be present in the feed to this reaction. Calculations will stop if it is present.

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METHANation reaction

The reactions are



Hydrocarbons other than methane will be considered as chemically inert but their presence will affect the reaction calculation as the second equation is not equimolar. Oxygen cannot be present in the feed or the calculation will stop.

SECOndary REFormeR

The reactions are the same as the METHANator but oxygen is allowed and is totally consumed producing CO, CO₂, H₂O, and CH₄ coexisting in equilibrium. Hydrocarbons other than methane will be considered as chemically inert. However, their presence will affect the reaction calculation as the second equation is not equimolar.

STEAm REFormeR

Hydrocarbons and any of the following components are allowed to react: CO, CO₂, H₂, H₂O, and O₂. The components will react and achieve thermal and mass equilibrium as in the METHANator. Any oxygen found in the input stream will be totally consumed.

NOTE: You are allowed to override the default heating values for petroleum fraction components involved in STEAm REFormeR calculations. See the **OPTIONAL COMMAND DETAILS** section for further information.

METHanol SYNthesis reaction

The reactions are $\text{CO(g)} + \text{H}_2\text{O(g)} = \text{CO}_2\text{(g)} + \text{H}_2\text{(g)}$ and $\text{CO(g)} + 2\text{H}_2\text{(g)} = \text{CH}_3\text{OH(g)}$

Components other than methanol are allowed and will be treated as chemically inert. However, they will affect the reaction calculation as the second equation is not equimolar.

AMMonia SYNthesis reaction

The reaction is: $\text{N}_2\text{(g)} + 3\text{H}_2\text{(g)} = 2\text{NH}_3\text{(g)}$

Other components are allowed but they will be treated as chemically inert. However, their presence will affect the reaction calculation as it is not equimolar.

Reactor: Stoichiometric Reaction Commands

The stoichiometric reactor type calculates component distribution using key component conversion and stoichiometric numbers for products and reactants. A heat of reaction (per mole of key component converted) can be specified. A component is specified as the LIMiting reactant and the CONversion of that component is also specified. If the flowrate of one of the reactants becomes negative, the CONversion of the LIMiting reactant will be reduced until the negative flowrate is zero. Enter all of the following commands to specify a simple reactor.

LIMiting reactant =

Enter the component ID number for key component.

CONversion =

Enter fractional conversion of key component.

STOichiometric COEfficients =

The STOichiometric COEfficients for the reactants (enter as negative numbers) and the products (enter as positive numbers) are specified. For components not affected by the reaction, STOichiometric COEfficients are entered as zero. All coefficients for the components must be coded in the same order as their component ID numbers on the COMponent command in the GENeral section.

NOTE: Fractional stoichiometric coefficients may be entered. The values must be preceded by a 0. E.G. STO COE = 0, 0.0, -1, 0, -0.5, 0.5.

HEAt of reaction (H units/molar Q units) =

Enter the heat of reaction per mole of key component converted. Enter a **negative** number if the reaction is exothermic. This heat of reaction is based on ideal gas at 32 F and 1 atmosphere. This command is optional but highly recommended for the simple reactor.

Reactor: Heat of Formation Table Commands

For all the specific reaction types, you should choose either the JANAF Thermochemical Tables or the NATional Bureau of Standards data to describe the chemical equilibria. This command is not valid for the *stoichiometric reaction type*.

(select only one)

NATional data

National Bureau of Standards Thermochemical Table is used to calculate heats of formation. This is the default.

JANaf data

Joint Army, Navy, and AirForce Thermochemical Table is used to calculate heats of formation.

NOTE: Operating temperature for each reactor should not exceed 3800 F (2093.3 C) if you use JANAF data or 2200 F (1204.4 C) if you use National Bureau of Standards data.

Reactor Optional Command Details

Reactor: Optional Steam Reformer Commands

For STEam REFormer reactions involving petroleum fractions, you may wish to override the default heating values which will be calculated by DESIGN II. Any of three commands can be entered in the GENeral section of your input file to override the default heating values for petroleum fraction components involved in STEam REFormer calculations.

HIGH HEAting value (H units / Q units) i =

Enter desired high (wet) heating value for petroleum fraction "i", where "i" is the component ID number.

LOW HEAting value (H units / Q units) i =

Enter desired low heating value for petroleum fraction "i", where "i" is the component ID number.

CARbon to **HYD**rogen weight ratio i =

Enter the desired value for petroleum fraction "i", where "i" is the component ID number. The heating value is calculated by DESIGN II for petroleum fraction components using the CARbon to HYDrogen weight ratio. 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.

Reactor: Temperature Approach Commands

You should determine if the default temperature of approach value is reasonable for your simulation. If it is not, you can enter appropriate values for the temperature of approach for specific reactions. The other approach is to use the PROducts commands to describe the behavior of the equilibrium reactor.

The outlet temperature, pressure and composition can be obtained from plant data or catalyst vendor information. These conditions are used only to determine a temperature of approach for a particular reactor and catalyst. They do not necessarily have to be identical to the conditions in a DESIGN II simulation of this reactor.

TEMperature **AP**proach **COSHIF**t (T units) =

Enter the desired temperature of approach for the COSHIFt reaction. Can be used for all reactions except AMMonia SYNthesis. Default is 0 F.

TEMperature **AP**proach **METHAN**ation (T units) =

Enter the desired temperature of approach for the METHANation reaction. Can be used with reactions for METHANation, SECondary REFormer, and STEam REFormer. Default is 0 F.

TEMperature **AP**proach **METHanol SYN**thesis (T units) =

Enter the desired temperature of approach for the METHanol SYNthesis reaction. Only used with the METHanol SYNthesis reaction. Default is 0 F.

TEMperature **AP**proach **AMMonia SYN**thesis (T units) =

Enter the desired temperature of approach for the AMMonia SYNthesis reaction. Only used with the AMMonia SYNthesis reaction. Default is 0 F.

NOTE: Temperature of approach (of a certain reaction) is defined as the difference between the actual exit stream temperature of the actual reactor and the temperature at which the reactor product composition would be in equilibrium. The temperature difference can sometimes have a negative value.

The temperature of approach can also be determined by using the three PROduct commands below.

PRO for **TEM AP** determination (molar Q units/t units) =

Enter the product stream compositions in the same order as the COMponent list in the GENeral section. DESIGN II will determine the temperature deviations from the product temperature.

PROduct **TEM**perature (T units) =

Enter the product temperature.

PROduct **PRE**ssure (P units) =

Enter the product pressure.

Reactor: Optional Commands

DUTy (H units/t units) =

Enter the total duty for the reactor. Default is zero.

DELta pressure (P units) =

Enter the pressure drop in the reactor. Default is zero.

TEMperature **OUT GUE**ss (T units) =

Enter a guess for the reactor outlet temperature. This command is used primarily for adiabatic reactions. Default is 60°F.

For reactors using specific reactions, HEAt of FORmation at 25C must be supplied for every component with an ID number greater than 99. You can use the following GENeral section commands to enter this data.

HEAT of **FOR**mation (H units/molar Q units) i =

Enter the heat of formation for component "i", where "i" is the component ID number.

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or

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.

Reactor: Lost Work Commands

If you have entered a LOST work command in the GENeral section, several commands should be considered for the REActor portion of the analysis. You have the option of setting the exchange temperature to be used for a REActor calculation for which ISOthermal, TEMperature OUT, or DUTy has been specified.

TEMperature of **EX**change (T units) =

Enter value for exchange temperature for the utility side of the calculation. Default is 250F.

The LOST work calculation requires heat of formation and entropy of formation for each component in the process when a reactor module is used. These data are automatically available for components 1-99 from the pure component data base. For components with ID numbers greater than 98, use the following command to enter entropy of formation data. Use the HEA FOR command listed above in the Optional Command section to enter heat of formation data for components greater than 98.

ENTropy of **FOR**mation (H units/molar Q units/T units) i =

Enter the entropy of formation for component "i", where "i" is the component ID number. The allowable units are:

BTU/LBMOL/R (default) KCAL/KGMOL/K CAL/GMOL/K J/GMOL/K KJ/KGMOL/K

For example,

```
GENeral,  
  COMponents = 2,49,48,62,1021,  
  ENTropy of FORmation (BTU/LBMOL/R) 1021 = -30.9907,  
  HEAt of FORmation (BTU/LBMOL) 1021 = -86544,
```

Reactor Command Summary

Reactor Type

ADiabatic reactor
ISOthermal reactor
TEMperature OUT (T units) =

Specific Reaction Type Commands

COSHIFt reaction
METHANation reaction
SECondary REFormer
METhanol SYNthesis reaction
AMMonia SYNthesis reaction

Stoichiometric Reaction Commands

LIMiting reactant =
CONVersion =
STOichiometric COEFFicient =
HEAt of reaction (H/molar Q units) =

Heat of Formation Table Commands

(Specific Reactions only)

NATional data
JANaf data

Optional Steam Reformer Commands

HIGH HEating value (H units / Q units) j =
LOW HEating value (H units / Q units) j =
CARbon to HYDrogen weight ratio i =

Temperature Approach Commands

TEMperature APProach COSHIFt (T units) =
TEMperature APProach METHANation (T units) =
TEMperature APProach METhanol SYNthesis (T units) =
TEMperature APProach AMMonia SYNthesis (T units) =
PROduct for TEMperature APProach (molar Q/t units) =
PROduct TEMperature (T units) =
PROduct PREssure (P units) =

Optional Commands

DUTy (H units/t units) =
DELta pressure (P units) =
HEAt of FORmation (H units/molar Q units) i =

Lost Work Commands

TEMperature of EXChange (T units) =
ENTropy of FORmation (H units/molar Q units/T units) i =

Thermodynamic Commands

HKEy =
KKEy =
DKEy =

Reactor Step by Step

Reactor STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
Equipment number
Equipment name

REA
Assigned equipment flowsheet number
User choice - up to 16 characters

Inlet stream	Unlimited in number
Outlet streams	One or two; if two, 1st is vapor, 2nd is liquid (two only for stoichiometric reactor)

Reactor STEP 2

Choose a specific reaction type or a stoichiometric reaction. Enter ONE of the following:

Adiabatic reactor (default)	ADI
Isothermal reactor	ISO
Reactor product temperature out	TEM OUT (T units) =

Reactor STEP 3

Choose a specific reaction type OR a stoichiometric reaction. Enter ONE of the following;

CO shift reaction (reaction is: $\text{CO(g)} + \text{H}_2\text{O(g)} = \text{CO}_2\text{(g)} + \text{H}_2\text{(g)}$ Oxygen is not allowed)	COSHIF
Methanation reaction (reactions are $\text{CO(g)} + \text{H}_2\text{O(g)} = \text{CO}_2\text{(g)} + \text{H}_2\text{(g)}$ $\text{CO(g)} + 3\text{H}_2\text{(g)} = \text{CH}_4\text{(g)} + \text{H}_2\text{O(g)}$ Oxygen is not allowed)	METHAN
Secondary reformer reaction (reactions are the same as the METHANator but oxygen is allowed and is totally consumed producing CO, CO ₂ , H ₂ O and CH ₄ coexisting in equilibrium)	SEC REF
Steam reformer reaction (hydrocarbons and any of the following components are allowed to react: CO, CO ₂ , H ₂ , H ₂ O and O ₂)	STE REF
Methanol synthesis reaction (reactions are $\text{CO(g)} + \text{H}_2\text{O(g)} = \text{CO}_2\text{(g)} + \text{H}_2\text{(g)}$ and $\text{CO(g)} + 2\text{H}_2\text{(g)} = \text{CH}_3\text{OH(g)}$)	MET SYN
Ammonia syntheses reaction (reaction is $\text{N}_2\text{(g)} + 3\text{H}_2\text{(g)} = 2\text{NH}_3\text{(g)}$)	AMM SYN

Stoichiometric reaction (enter the following)

Component ID number for key component	LIM =
Fractional conversion of key component	CON =
Coefficients for each component in the order listed on the COMponents command in the GENeral section (enter positive numbers for products, negative numbers for reactants and zeroes for components not entering into the reaction)	STO COE =
and, optionally,	

Heat of reaction per mole of key component converted (enter a negative number if the reaction is exothermic)	HEA (H units/molar Q units) =
--	-------------------------------

Reactor STEP 4

Choose heat of formation data for specific reaction types only. Does not apply to stoichiometric reactions. Heat of formation data table specification (enter ONE of the following)

National Bureau of Standards thermochemical Table (default)	NAT
JANAF Thermochemical Table	JAN

Reactor STEP 5

Choose an optional temperature approach specification for specific reaction types. Does not apply to stoichiometric reactions (select ONE of the following)

Temperature of approach for the COSHIFt reaction (can be used for all reactions except AMMonia SYNthesis; default is 0 F)	TEM APP COSHIF (T units) =
Temperature of approach for the METHANation reaction (can be used with reactions for METHANation, SECondary REFormer, and STEam REFormer; default is 0 F)	TEM APP METHAN (T units) =
Temperature of approach for the METHanol SYNthesis reaction (can only be used with the METHanol SYNthesis reaction; default is 0 F)	TEM APP MET SYN (T units) =
Temperature of approach for the AMMonia SYNthesis reaction (can only be used with the AMMonia SYNthesis reaction; default is 0 F)	TEM APP AMM SYN (T units) =

General temperature approach specification (enter ALL of the following three commands)

- Product stream compositions in the same order as the COMponent list in the GENeral section	PRO TEM APP (molar Q units/t units) =
- Product temperature	PRO TEM (T units) =

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- Product pressure

PRO PRE (P units) =

OPTIONAL - Choose any of the optional commands listed below.

STeam REFormer reaction heating value changes (choose any of the following)

High heating value where "j" is the component ID number (place command in the GENeral section)

HIG HEA (H units/Q units) **j** =

Low heating value where "j" is the component ID number (place command in the GENeral section)

LOW HEA (H units/Q units) **j** =

Carbon to hydrogen weight ratio where "i" is the component ID number (place command in the GENeral section)

CAR HYD i =

Additional component specification for COMponents numbers greater than 98

Heat of formation for component "i" where "i" is the component ID number (place command in the GENeral section)

HEA FOR (H units/molar Q units) **i** =

Reactor duty and pressure drop specifications (select ANY of the following options)

Pressure drop in the reactor (default is zero)

DEL (P units) =

Total duty for the reactor (default is zero)

DUT (H units/t units) =

IF LOST work command in GENeral section THEN select

Value for exchange temperature for the utility side of the calculation (enter only if ISO, DUT or TEM OUT commands are used; default is 250 F)

TEM EXC (T units) =

Entropy of formation where "i" is the component ID number (place command in the GENeral section)

ENT FOR (H units/molar Q units/T units) **i** =

NOTE: The allowable units for ENT FOR are:

BTU/LBMOL/R (default)

J/GMOL/K

KCAL/KGMOL/K

KJ/KGMOL/K

CAL/GMOL/K

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

HKE =

Density option

DKE =

Reactor Examples

There are several sample flowsheets in "Chapter 39: Reactor Samples - c:\designii\samples\equipmnt\reactor" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 36: Refine Column

The REFine module is used for rigorous simulation of distillation columns receiving high hydrocarbon-content feeds. Many common refinery units can be modeled, including preflash towers, atmospheric columns, vacuum columns, FCC main fractionators and quench columns. Side strippers, pumparounds, and feed furnaces can be added to the main column configuration for a rigorous, simultaneous calculation.

This module can be used for designing, modifying refinery fractionators with very good results. It is possible to duplicate the operation of existing units within a few percent of actual plant data.

Many important operational parameters can be matched, such as tower temperatures, reflux, product rates, and property specifications. Significant discrepancies are usually due to inaccuracies in data collection but may be due to operational problems. In these cases, REFine may be used to identify the source of the problem and determine the solution.

Refine Distillation Columns Features

Column Types

Five major column types encompass all common refinery fractionators distinguished by the reflux generation and condenser type. All associated operations (reboil, stripping, pumparounds, etc.) are available within each column and multi-column operations are permitted.

The REFine module offers a great deal of flexibility in the definition of column parameters. You are allowed an essentially unlimited number of stages, side strippers, pumparounds, heaters/coolers, products, feeds to the main column, steam feeds, feed furnaces, water decants, and components. REFine uses theoretical trays, i.e. equilibrium stages, therefore when simulating existing plants it is necessary to estimate tray efficiency in each column section to determine the number of equilibrium stages for the model.

Product Specification and Column Control

The REFine module allows you to control the fractionation process in several ways. You can directly specify product rates or qualities such as end points, letting the program adjust product rates to meet your specifications (see the ***Refine: Specification Commands*** section for details). You can also use FIX commands to set column temperatures, vapor rates and liquid rates to desired values by varying other parameters (see ***Refine: FIX Tray Conditions*** section).

Calculation Technique

The REFine module uses a unique mathematical approach which simultaneously calculates heat/material balance for a main column, side strippers and pumparounds. By treating these separate units as if they were a single column, the rigorous calculations are completed significantly faster than other available crude unit programs. In addition, accurate results can be achieved using data that is typically available to you because the REFine module has a great deal of flexibility in specifications and column description.

Water K-values and Decant

The REFine calculation technique also handles water in a completely rigorous manner with water automatically decanted at the condenser and free water at tray conditions producing warnings if present. For quench or other columns where several trays may have large amounts of free water present, water decants can be added as needed. The pumparounds can be pure water or water-hydrocarbons. Water solubility in hydrocarbons is taken into account for each product.

Stream Order

Certain conversions must be followed when defining feed and product streams in the REFine module.

- Each feed stream to the REFine module is assigned a unique number. The feed stream numbers are listed in top-to-bottom order. Steam feeds are NOT numbered streams.
- Each product stream is assigned a unique number.

The product stream numbers are given negative signs and listed in top-to-bottom order. A decant stream from the condenser is NOT a numbered product stream but any water decant streams from trays are numbered product streams.

- Internal streams, such as pumparound draw and return streams, side stripper draw and return streams, reboiler streams, or reflux streams are not numbered. Their compositions, flow rates and other properties are automatically estimated and calculated values are reported in the column output.

Tray Numbering Convention

Certain conventions must be followed when numbering trays in the REFine module. In REFine there is a distinction between "stages" and "trays". The total number of "stages" for the main column and separate values for each side stripper are specified. Tray numbers are used to locate feeds, side draws, side heater/coolers, pumparounds, and side strippers.

- "Stages" refers to the total number of theoretical trays plus partial condenser and reboilers, if present. "Stages" does NOT include total condensers.
- "Trays" are theoretical trays and reboilers.

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All locations refer to tray locations. Number the trays (including any reboilers) in top-to-bottom order starting with the main column. Tray 1 is the top tray of the main column. Tray 0 is the condenser, if present.

Step-by-Step Procedure

Specifying a REFine column simulation with DESIGN II is a step-by-step procedure and is summarized below:

- Select REFine module, assign equipment number, name, inlet streams and outlet streams.
- Define the column type by selecting the arrangement of reflux and overhead product.
- Add any required column configuration commands.
- Determine the number of heat and material specifications required based on the column type and select the one(s) for your simulation.
- Add any side draws, strippers, and water decants with the appropriate specifications.
- Add heat sources (steam, reboiler, or vapor feed). Required at the **bottom** of each column.
- Add any pumparounds and associated specifications.
- Add optional tray "FIXes" and product property specifications.
- Add optional commands as needed for cooling curves, print control, column sizing, and more.
- Add restart commands, if you have several cases to run.

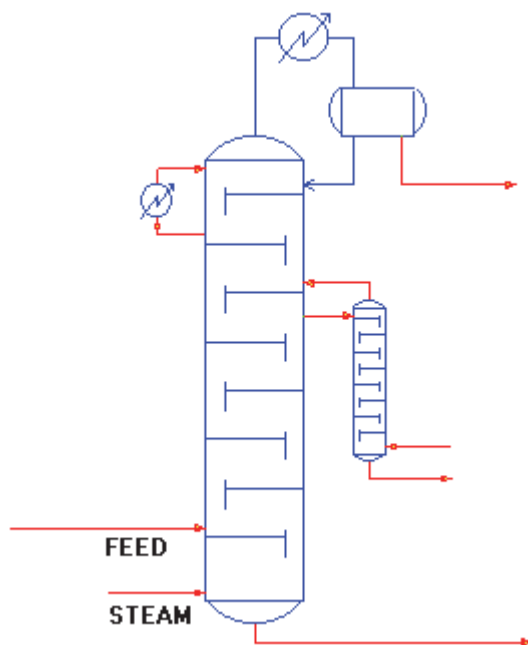
Refine Distillation Columns Command Details

Refine: Column Type

Five column types are available in the REFine module. These are differentiated by the combination of reflux generation and overhead products. Reflux is generated either internally (top tray pumparound) or externally (condensed overhead vapor returned to top tray). Overhead products can be produced as vapor, liquid or both.

The main column is of primary concern, with each type permitting an essentially unlimited number of associated operations (side draws, strippers, pumparounds, feeds, feed heaters, etc.). Select the appropriate column type below:

TOTAL condenser

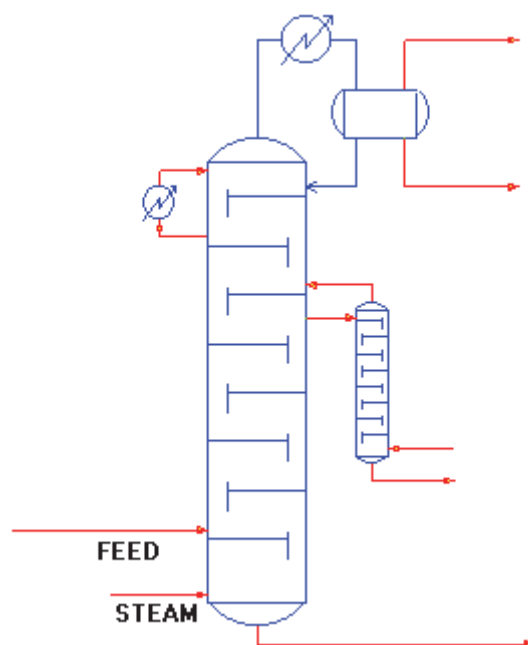


This is an externally refluxed column. Reflux returning to the top tray includes any water dissolved in the hydrocarbons. Any remaining water in the condenser is automatically decanted.

Selection Criteria

- EXTERNAL REFLUX
- NO OVERHEAD VAPOR

PARTial condenser

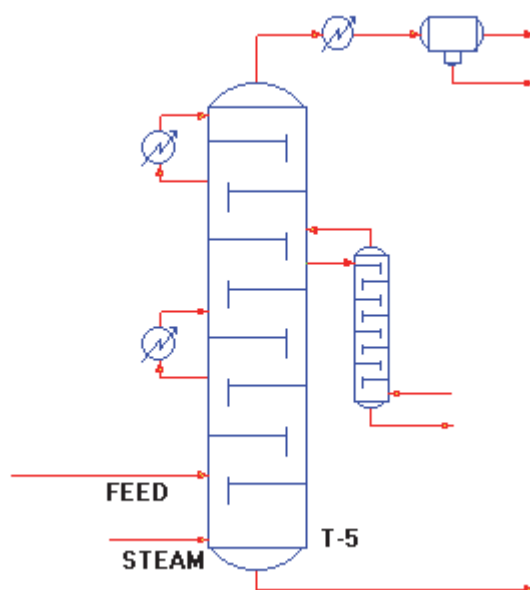


This is an externally refluxed column which decants water (if it is present in sufficient quantity) as a separate liquid phase. Solubility of water in liquid hydrocarbons is taken into account for both the liquid distillate and the reflux returning to the column. The vapor distillate will be saturated.

Selection Criteria

- EXTERNAL REFLUX
- OVERHEAD VAPOR AND LIQUID PRODUCTS

PUMparound with TOTal condenser (internal reflux)



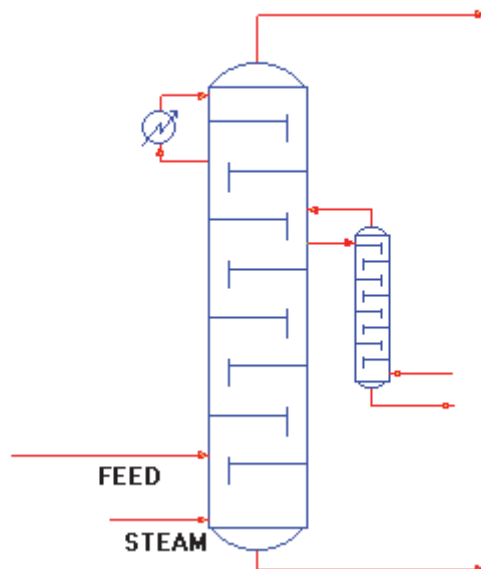
This internally refluxed column has a top tray pumparound to generate reflux. There is no liquid returned from the external condenser to the main column. Water, if present, is decanted automatically from the external condenser.

Selection Criteria

- INTERNAL REFLUX (Top pumparound on Tray 1)
- NO VAPOR PRODUCT

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PUMparound REFlux (internal reflux, no condenser)

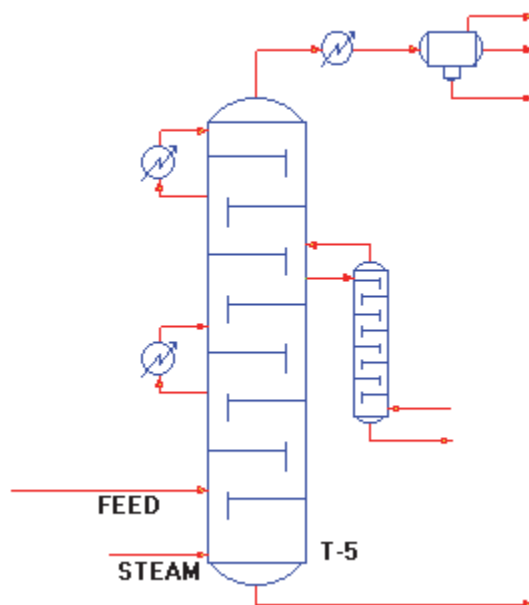


This internally refluxed column has no overhead condenser to provide reflux. Instead, a pumparound on tray 1 generates internal reflux. With this column type, there is no automatic decant of liquid water.

Selection Criteria

- INTERNAL REFLUX (top pumparound on tray 1)
- NO OVERHEAD LIQUID PRODUCT

PUMparound with PARTial condenser (internal reflux)



This column has a top tray pumparound to generate reflux, and an external partial condenser. There is no liquid returned to the column from the partial condenser. Water (if present) is decanted automatically from the condenser.

Selection Criteria

- INTERNAL REFLUX (top pumparound on tray 1)
- BOTH VAPOR AND LIQUID PRODUCTS

Refine: Selecting of Column Types for Special Applications

Condensers with no liquid product

Of the main column types, PUM REF most closely approximates a column with a partial condenser, where all condensed liquids are returned as reflux. The top tray of the PUM REF becomes the "condenser".

Hot Condensers

If you have a partial condenser column which has a hot condenser (200 F+) and the column is steam stripped, the PUM REF column type will be easier to converge. Specify the "condenser" temperature by using a FIX TEM command for tray 1. Be careful when locating the feed, pumparounds, and strippers as tray 1 is your condenser in the PUM REF option. Use a PREssure PROfile command, if desired, to simulate the drop in pressure from tray 2 to tray 1 (condenser pressure drop). See the *Refine: Profiles Which are Set Values* section for details.

This can be extended to the two drum overhead system where the first (hot) drum acts as a reflux condenser. Use the PUM REF column type to obtain the first converged solution (with a whole vapor product). Then switch to a PUM PAR with the external condenser acting as the "cold" product separator. When switching remember to re-check all location and profile commands and carefully select the appropriate heat and material balance specifications.

Compound Condensers

The PUM TOT column type can be used to simulate a compound condenser if there is no water decant in the first (internal) condenser.

Absorbers and Reboiled Absorbers

The PUM REF column type is the closest approximation to an absorber or reboiled absorber in the REFine module. To simulate an absorber, you must have a liquid feed to tray 1 and a vapor feed (or steam) below the bottom tray. Do not enter a PROduct rate command. Do enter a PROduct rate GUEss command to generate initial vapor and liquid profiles. The top tray pumparound duty should be set to a very small value.

For a reboiled absorber, add a REBoiler command to specify reboiler duty. A liquid feed to tray 1 is required. Any other feeds are optional. Reboiler commands are given in the *Refine: Reboilers* section.

Quench Columns

The PUM REF is the column option most often chosen to model the quench section of a distillation column. A **P-S** command (see *Refine: Profiles Which are Initial Estimates Only*) for water partial solubility is required for modeling columns where significant amounts of free water will be found on the trays, or for water pumparounds and water decants from trays other than the condenser.

Refine: Required Column Description

All the commands in this section are required for all column types.

The commands provide the following basic column description:

- Number of equilibrium stages
- Temperature guesses for the top and bottom products
- Pressure of the columns
- Feed tray locations

Number of Equilibrium Stages

STAges =

Enter the number of equilibrium stages for the main column followed by the number of stages in any side strippers, beginning with the top stripper. Minimum of three stages for the main column. (example: STA=25,3,3)

A reboiler (if present) is a theoretical stage and must be counted, both for the main column and for side strippers. The partial condenser is a theoretical stage and must be counted as a stage but a total condenser is not counted as a stage. Therefore PAR and PUM PAR column types include the condenser in the number of stages but TOT and PUM TOT do not include the condenser.

Only the STAg_{es} command refers to equilibrium stages; all location commands refer to trays, see Feed Tray Locations below.

Column Temperatures

TEMperature of **TOP** (T units) =

Enter your initial estimate for the top tray temperature for main column. Optionally, you can enter guesses for the top tray temperature for each stripper column in top-to-bottom order

TEMperature of **BOT**tom (T units) =

Enter your guess for bottom product temperature. Optionally, you can enter guesses for the bottom tray temperature for each stripper column in top-to-bottom order.

Column Pressures

PREssure of **TOP** (P units) =

Enter the top main-column pressure. Following this number, you can also enter top-tray pressures for each side-stripper column in top-to-bottom order, but these are not required. If you do not specify side-stripper pressures, the program uses draw tray pressures.

DELta pressure (P units) =

Enter the pressure drops for the main column and then for each side stripper in top-to-bottom order. Without this command, pressure drop is assumed to be zero in the main column and side strippers.

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REFine assumes a linear pressure profile. You also have the option to specify nonlinear profiles with a PREssure PROfile command (see *Pressure Profile*).

Feed Tray Locations

LOCation of FEEds =

Enter the *tray* numbers where feeds enter the column, in top-to-bottom order corresponding to the feed stream numbers on the REFine module command. The liquid portion of a feed mixes on the feed tray and the vapor portion of a feed mixes on the tray above the feed tray.

All locations (feeds, pumparounds, strippers, etc.) refer to *tray* locations. To determine tray locations, number the trays (including any reboilers) in top-to-bottom order starting with the main column then each side stripper. Tray 1 is the top tray of the main column. Tray 0 is the condenser, if present.

Refine: Heat and Material Balance Specifications

Having defined the basic column configuration and operating parameters, the user controls the simulation using heat and material balance specifications. There is a large number of specifications from which to choose. A user may choose to specify an item for many reasons:

- confidence in a particular measured data point
- requirement to achieve a particular rate
- requirement not to exceed a known practical plant constraint

IMPORTANT: The column can be further controlled with the FIX and PROduct SPECification commands. See the sections *Refine: FIX Tray Conditions* and *Refine: Product Property Specifications*.

To specify the REFine column follow these three steps.

1. First determine the required number of specifications based on the column type from the table in *Refine: Column Type Versus Number of Specifications Required*
2. Then simply enter the required number of specification commands from the choices detailed in *Refine: Specification Commands* REFine will automatically determine what column parameters to vary to meet your choice of specifications.

If more than the required number of specifications for your column type are entered, then the specifications used will be based on the hierarchy of commands and the other entered commands will be used as initial guesses. The hierarchy of commands for each column type is given below in the section *Refine: Hierarchy of Heat and Material Balance Specifications*

Refine: Column Type Versus Number Of Specifications Required

Based on column type choose the number of specifications required and the commands allowed.

		Allowable specifications X						
Column Type	Number Req'd	PRO	DUT	REF	TEM CON	PRO OVE	HEA PUM	FIX TEM
TOT	1	X	X	X				
PAR	2	X	X	X	X	X		
PUMTOT	1	X	X				X	X
PUMPAR	2	X	X				X	X
PUMREF	1	X					X	X

Refine: Specification Commands

Enter the required number of specification commands from the list below.

If your column type requires two specifications, choose the combination carefully. Certain specifications are difficult to achieve either through the magnitude of the parameter (such as small overhead vapor flow versus large bottom draw rate) or interconnection between parameters (such as overhead vapor and liquid rates, or condenser temperature and condenser duty).

PROduct rate (option, Q units/t units) =

Enter rates for unstripped products from the main column in top-to-bottom order, use zeros for unspecified flowrates to maintain order. Products include vapor distillate (PAR, PUM PAR, and PUM REF), liquid distillate (TOT, PAR, PUM TOT, and PUM PAR), unstripped side draws (including "free water" tray draws, not including condenser decant) and bottom product. At least one of the vapor distillate, liquid distillate or bottom flowrates must be zero. All volumetric and weight PROduct rate and PROduct OVERhead specifications are on a dry basis. Volumetric and weight product rate specifications can not be specified on a wet basis. The default molar PROduct specification is on a wet basis. You may add the keyword DRY to give molar product rates on a dry basis.

PRO (DRY, KGMOL/HR) $i = 0, 1575, 472.7$

PRO STR (DRY, KGMOL/HR) = 125, 320, 92

Flowrates for unstripped side draws are always required. Nonzero values of vapor distillate, liquid distillate, and bottoms distillate are used as specifications depending on the hierarchy of specifications for your column type (see Hierarchy of

Heat and material Balance Specifications). More information on this command follows later in this section.

PROduct rate **GUE**ss (molar Q/t units)=

If you enter any PROduct rates in mass or volume units, you should also enter rate estimates for those products in *molar* units with a PROduct rate GUEss command. This is NOT a specification, only a guess. REFine automatically performs FENske calculations to estimate molar rates if this command is not entered.

DUTy of condenser (H units/t units)=

Enter the duty required to condense hydrocarbon product, and any water present. Water is automatically decanted.

REFlux ratio =

Enter the molar reflux ratio for the main column. Reflux is defined as moles of liquid returned to the column divided by the overhead molar product rate(s).

TEMperature of **CON**denser (T units) =

Enter the exit temperature of the condenser (accumulator temperature).

PROduct **OVE**rhead rate (Q units/t units)=

Use this command *only* to enter total distillate product when you have also entered a TEMperature of CONdenser specification (which will determine the vapor/liquid split). Volumetric and weight product rate specifications will always be on a dry basis. The default molar PROduct specification is on a wet basis. You may add the keyword, DRY, to specify molar product rates on a dry basis. E.G. PRO OVE (DRY, KGMOL/HR) = 1480.

If the value for **PRO OVE** was entered using mass or volume units, you must enter a molar guess.

PROduct **OVE**rhead **GUE**ss (mole Q/t units) =

HEAT from **PUM**paround (H units/t units)=

Enter the amount of heat removed by the top pumparound. Details are given in the Pumparounds section.

FIX TEMperature of top tray (T units)=

For internally refluxed columns, you can use this command to force the tray temperature to a specified value by varying the bottom product rate. The column heat balance will be satisfied by adjusting the top tray pumparound duty. This command overrides all other heat/material balance commands.

Refine: Hierarchy of Heat and Material Balance Specifications

If more than the required number of specifications is entered, the specifications used are those highest in the hierarchy of commands listed below. The other commands, entered but not used as specifications, will be used as initial guesses.

Hierarchy for **TOTAL** condenser column types

One specification is allowed for TOT column types. If more than one is entered, the command highest in the list below is used.

Specifications	Command Example
Condenser duty	DUT y =15E6
Liquid distillate rate	PRO duct = 150, 0
Bottom product rate	PRO duct = 0, 2000
Reflux ratio	REF lux RAT io = 3.5

Hierarchy for **PUM**paround with **TOTAL** condenser column types

One specification is allowed for PUM TOT column types. If more than one is entered, the command highest in the list below is used.

Specification	Command Example
Fix temperature of top tray	FIX TEM perature 1 = 100,1,1
Liquid distillate rate	PRO duct = 3000, 0
Bottom product rate	PRO duct = 0, 1000
Heat from top pumparound	HEAT PUM paround = 15E6

Hierarchy for **PUM**paround with internal **REF**lux column types

One specification is allowed for PUM REF column types. If more than one is entered, the command highest in the list below is used.

Specifications	Command Example
Fix temperature of top tray	FIX TEM perature 1 = 100,1,1
Vapor distillate rate	PRO duct = 2000, 0
Bottom product rate	PRO duct = 0, 5000
Pumparound duty	HEAT PUM paround = 30E6

Hierarchy for **PART**ial condenser column types

The **PART**ial condenser column requires two heat/material balance specifications from the following:

Specifications	Command Example
Condenser duty	DUT y = 3E6
Liquid distillate rate	PRO duct = 0, 75, 0
Vapor distillate rate	PRO duct (LB/HR) = 5000,0,0
Bottom product rate	PRO duct (BBL/DAY) = 0, 0, 10000
Reflux ratio	REF lux RAT io = 4

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Condenser temperature
Total overhead product
and
Condenser temperature

TEMperature CONdenser = 120or
PROduct OVerhead (BBL/DAY) = 1500

TEMperature CONdenser = 100

If you enter more than two specifications, REFIne will use the combination that is highest on the following list.

condenser duty-liquid distillate rate
condenser duty-reflux ratio (requires PRO GUE or VAP PRO)
condenser duty-bottom product rate
condenser duty-vapor distillate rate
liquid distillate rate-reflux ratio
liquid distillate rate-vapor distillate rate
liquid distillate rate-bottom product rate
vapor distillate rate-reflux ratio
vapor distillate rate-bottom product rate
bottom product rate-reflux ratio
condenser temperature-reflux ratio (requires PRO GUE or VAP PRO)
condenser temperature-bottom product rate
condenser temperature-total overhead product rate (liquid plus vapor distillate)

Hierarchy for PUMparound with PARTial condenser column types

The PUM PAR column requires two heat/material balance specifications from the following:

Specification	Command Example
Fix temperature on top tray	FIX TEMperature 1 = 100,1,1
Liquid distillate rate	PROduct = 0, 275, 0
Vapor distillate rate	PROduct = 75,0,0
Bottom product rate	PROduct (BBL/DAY) = 0, 0, 10000
Condenser duty	DUTy = 15E6
Top pumparound duty	HEA PUM = 42E6
Condenser temperature	TEMperature CONdenser = 120or
Total overhead product rate and Condenser temperature	PROduct OVerhead (BBL/DAY) = 1500 TEMperature CONdenser = 150

If you enter more than two specifications, REFIne will use only the combination that is highest on the following list.

EXCEPTION: A FIX TEMperature of top tray command overrides all other heat/material balance commands.

liquid distillate rate-vapor distillate rate
liquid distillate rate-bottom product rate
liquid distillate rate-top pumparound duty
vapor distillate rate-bottom product rate
vapor distillate rate-top pumparound duty
bottom product rate-condenser temperature
top pumparound duty-condenser temperature
bottom product rate-condenser duty
top pumparound duty-condenser duty
total overhead product rate-condenser temperature

Refine: Notes on Specifications

Specifying Product Rates

The PROduct rate command is used to enter vapor distillate, liquid distillate, unstripped side draws and bottom product rates. For the PARTial and PUM PAR condenser columns, you must always enter values for all three, even if two are entered as zero. The first entry is for vapor distillate, the second is for liquid distillate and after side draws, the last entry is for bottoms rate.

For TOT and PUM TOT columns, the vapor distillate is omitted and in PUM REF the liquid distillate is omitted. Either top or bottom product rate must be left as ZERO to allow the program to calculate the overall material balance.

NOTE: Any *unstripped* side draw product rates are entered in top-to-bottom order preceding the bottoms rate. Product flowrates from side strippers are specified using commands given in the *Refine: Side Strippers* section.

Nonmolar product rates are entered on a dry (water-free) basis. If you specify flowrates in *molar* units, you must include the water of saturation (decanted water is not included). For vapor products, the saturated water can be significant. It is best to specify the bottoms product rate and let the vapor product rate be calculated by mass balance. Normally, product rates entered on a molar basis include water of saturation. You may add the DRY keyword in the dimensional unit section of the PROduct command to indicate the values are on a dry basis.

PRO (DRY, LBMOL/HR) = 1000, 250, 0

For TOTal and PUM TOT condenser columns, all products are liquid. Liquid products are for the hydrocarbon-rich phase only; neither soluble nor decanted water is included.

Flowrate Estimates in Molar Units

If possible, you should specify product flowrates in molar units (for example, LBMOL), because the program performs calculations in these units. When you specify product flowrates in mass or volume units, you may provide approximate molar equivalents using the PROduct rate GUEss command to aid the program in initial vapor and liquid set up.

```
PRO (BBL/DAY)=0,1000,5000
PRO GUE=100,200,250
```

Specifying Total Overhead Product Rate

For PARTial and PUM PARTial condenser columns, you can specify total distillate product rates with the PROduct OVERhead rate command, *if* you also enter a TEMperature of CONDenser specification. The program will then calculate the vapor/liquid split based on the condenser temperature you specify.

NOTE: This is the *only* case in which the PROduct OVERhead rate command is valid.

Specifying Temperature of Condenser

The TEMperature of CONDenser specification sets the temperature of the reflux accumulator. Your TEMperature of TOP guess is for the first tray in the column.

Specifying Reflux Rates

Reflux Ratio is:

For a **TOTAL** condenser:

$$\frac{\text{moles of liquid returned}}{\text{distillate rate in moles}}$$

For a **PARTIAL** condenser column:

$$\frac{\text{moles of liquid returned to top tray}}{\text{vapor + liquid distillates in moles}}$$

Although not a specification option for **PUM REF**, **PUM TOT**, **PUM PAR** columns reflux ratio in the results is defined as:

$$\frac{\text{net liquid leaving top pumparound draw tray in moles}}{\text{vapor leaving tray 1 (including steam) in moles}}$$

Using the FIX TEMperature Command with PUM REF, and PUM TOT

The easiest way to converge these column types is to use a FIX TEMperature command to set the top-tray temperature by varying the bottom product rate. The heat balance will be closed at tray 1. The top and bottom product rates will float until the correct composition and rate are leaving the top tray.

When you use the FIX TEMperature command to set the top-tray temperature, the value you enter for TEMperature of TOP should be for tray 2.

If you use FIX TEM, be sure the fixed temperature is high enough to prevent water (if present) from condensing at the top tray pressure because water is not automatically decanted from tray 1.

Details on FIX commands are given in the *FIX Tray Conditions* section.

Using the HEAt from PUMparound Command (for PUM REF, PUM TOT, and PUM PAR)

When you use a HEAt from PUMparound command to specify heat removed in the top pumparound, do not enter a PROduct rate command for the top or bottom product. You should enter a PROduct rate GUEss command to generate initial vapor and liquid profiles.

Refine: Easiest Specifications

The easiest specification(s) to converge each column type is described below.

For TOT column types

Bottom product rate with molar guesses if the specification is in mass or volume units.

For example:

```
PROduct (BBL/DAY) = 0, 5000
PROduct GUEss = 250, 50
```

For PAR column types

Condenser temperature and bottom product rate, especially if you enter a guess for the vapor distillate rate. For example:

```
TEMperature of CONDenser = 150
PROduct (BBL/DAY) = -300, 0, 10000
```

For PUM REF column types

Fix top tray temperature. For example:

```
FIX TEMperature 1 = 100,1,1
```

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For PUM TOT column types

Fix top tray temperature. For example:

```
FIX TEMperature 1 = 100,1,1
```

For PUM PAR column types

Condenser temperature and bottom product rate, especially if you also enter a guess for the vapor distillate rate. For example:

```
TEMperature of CONdenser = 150  
PROduct (BBL/DAY) = -300, 0, 10000
```

Refine: Difficult Specifications And Cautionary Notes

TOT column types

1. The TOTal column should be used with caution when feeds contain hydrogen or other light gases.

PAR column types

1. Two heat-balance specifications (for example, top pumparound duty and condenser temperature) are the most difficult combinations to converge. Whenever possible, combine two material balance specifications, or one material balance and one heat balance specification. EXCEPTION: The combination of vapor distillate rate and liquid distillate rate is very difficult to converge and should be avoided.
2. Condenser temperature and condenser duty cannot be used together as heat/material balance specifications.
3. If you enter TEMperature of CONdenser and PROduct OVERhead rate, it is advisable to enter your best guesses for the expected vapor/liquid split by specifying negative values with the PROduct rate command for the vapor distillate product. For example:

```
PRO OVE (BBL/DAY)=10000  
PRO (BBL/DAY)=-2500,0,0
```
4. If you enter TEMperature of CONdenser and any PROduct rates, it is advisable to also enter your best guess for either vapor or liquid overhead product rate. For example:

```
TEM CON=120  
PRO=0,-200,1000
```
5. If you are simulating a steam stripped PAR column with an essentially zero liquid distillate rate (all condensed liquid is returned to column as reflux), then the distillate liquid rate *must* be a specification. Bottoms rate is a good choice for the remaining specification. The best way to approach this particular column configuration is to obtain a converged run using the PUM REF main column. Then use the temperature and vapor profiles from that run to initialize the PAR run.

PUM PAR column types

1. Two heat-balance specifications (for example, top pumparound duty and condenser temperature) are the most difficult combinations to converge. Whenever possible, combine two material balance specifications, or one material balance and one heat balance specification.

EXCEPTION: The combination of vapor distillate rate and liquid distillate rate is very difficult to converge and should be avoided.

PUM REF column types

1. Because of large temperature differences between the top tray and the second tray (especially for vacuum columns), it is sometimes helpful to enter a temperature profile using the TEMperature PROfile command described in the *Refine: Profiles Which Are Initial Estimates Only* section.

NOTE: In PUM REF, PUM PAR and PUM TOT, the top pumparound is automatically assigned the internal condenser's calculated duty. This cannot be over-riden. This is due to the automatic internal condenser in PUM REF, PUM PAR and PUM TOT.

Refine Distillation Columns Optional Commands

Refine: Side Draws

REFine permits up to nine side draws to be specified with the LOCation of SIDedraw, LOCation of SIDEdraws for WATer, and the PROduct rate commands.

LOCation of SIDedraws =

Enter the tray numbers where unstripped side draws including water decants are located, in top-to-bottom order. Do not include water decanted from the condenser. Negative numbers indicate vapor draws. Side draw product flowrates are specified on the PROduct rate command with other main column products. The unstripped side draw flowrates can only be varied with the PROduct SPECification command.

LOCation of SIDedraws for WATer =

Enter the tray numbers where pure water is to be decanted. Enter zeroes for any sidedraw locations which are for hydrocarbon products. Estimates for the water decant rates are entered on the PROduct rate command with the other main column products.

Example:

PUM REF

LOCation **SIDe** = 3, 3, 8

LOCation **SIDe** **WATer** = 3, 0, 0

PRO = 0, 50, 450, 1250, 358

The main column has three unstripped side draws: a water draw from tray 3 and hydrocarbon draws from trays 3 and 8. Their flowrates will be specified with the **PROduct** rate command; the water draw flowrate will be an estimate.

NOTE: A total of 12 products are allowed from REFI columns. This includes products from the main column, including side draws, and stripper products.

Refine: Condenser

PREssure of **CONDenser** (P units) =

Enter the pressure out of the condenser for TOT, PUM TOT, PAR, and PUM PAR column types. Default is the top tray pressure will be the same as that specified with the **PREssure** of **TOP** command.

TEMperature of **CONDenser** (T units) =

Enter the desired condenser temperature for TOT or PUM TOT column types. If you enter a value higher than the calculated bubble point for the product, the product will exit at the calculated bubble point temperature.

TEMperature of **CONDenser** **SUB**cooling (T units) =

Enter the degrees of subcooling for the overhead product and reflux for TOT or PUM TOT column types.

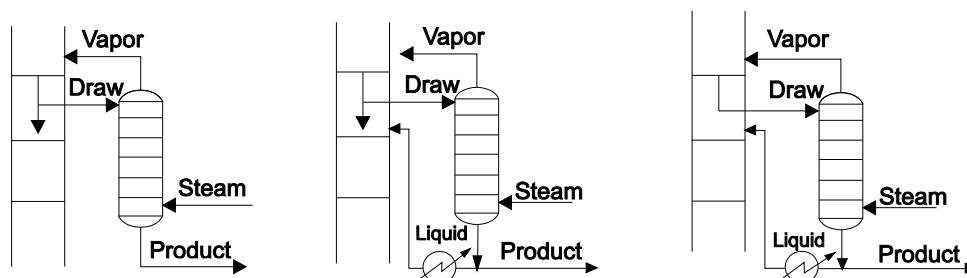
TEMperature of **CONDenser** **GUEss** (T units) =

Enter your guess for the condenser outlet temperature for TOT column types. The distillate product will leave at its bubble point temperature.

Refine: Side Strippers

Up to nine side strippers can be added to a column. Side strippers can be either reboiled or steam stripped but each must have a heat source. If reboiled, reboiler duties appear on the **REBoiler** command. If steam stripped, the steam description is given in the **STEam**, **LOCation** of **STEam**, **PREssure** of **STEam**, and **TEMperature** of **STEam** commands. The **STAg**es command includes number of theoretical trays and reboilers (if present).

There are three types of Side Stripper:



A. Partial draw with no liquid return

B. Partial draw with liquid return

C. Total draw with liquid return

Required Side Stripper Description

The side stripper column requires that the location of draw and return streams be specified. These commands must include entries for all side strippers.

LOCation of **DRAws** =

Enter the main column tray location of liquid draw from the main column to each stripper in top-to-bottom order.

LOCation of **VAPor** returns =

Enter the main column tray location for vapor return to the main column in top-to-bottom order. Remember that the vapor portion of all streams entering the main column rise up and mix with the tray *above* the specified tray location. Thus if you specify vapor return on tray 14, the vapor actually mixes on tray 13.

LOCation of **LIQuid** returns =

Enter the main column tray locations of liquid returned to the column (if present) from any side stripper. Enter zeroes for all strippers not having liquid returns to maintain top-to-bottom order.

NOTE: A total of twelve products can be specified for a Refine column. this includes products from the main column (including unstripped side draws and water decants) and stripper products.

Required Side Stripper Specifications

All side strippers require one or two heat and material balance specifications. Enter one or two specifications for all strippers according to the type of side stripper as given in the **Quick Reference Table** below. Enter zeroes to maintain top-to-bottom order.

PROduct from **STRipper** (Q units/t units)=

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Enter product flowrates from each stripper in top-to-bottom order. Normally, stripper product rates specified in mass or volume units are dry, while stripper product rates entered in molar units include water of saturation. Add the DRY command to indicate that stripper product rates in molar units are also dry.

PRO STR (DRY, KGMOL/HR) = 475, 370, 290.

DRAwrates to strippers molar Q units/t units or **FRA**) =

Enter the drawrates from the main column. You can specify either molar flowrates or the fraction of liquid drawn from the tray. A fraction of 1 implies total draw. If you use FRACTION units for one stripper, you must use it for all strippers.

RETurn flow from stripper (molar Q units/t units) =

Enter the molar rates for liquid returning to the main column from each stripper in top-to-bottom order. Enter zeroes for strippers which do not have liquid returns.

Optional Molar Product Guess

PROduct from **STR**ipper **GUE**ss (molar Q units/t units) =

If you have specified any product rates in mass or volume units, you may also enter estimates in molar units for those rates using this command.

Optional Return Liquid Cooling

Choose *one* of these three commands if you wish to specify the amount of cooling before the liquid is returned to the main column. Each liquid return can have one cooling specification. Enter zeroes to maintain correct top-to-bottom order.

HEAt from **RET**urn (H units/t units) =

Enter heat removal from each return liquid stream in top- to-bottom order.

TEMperature of **RET**urn (T units) =

Enter the temperature of liquid streams returning to the main column. If your specification is higher than the bubble-point temperature of the product stream, no heating will occur and the temperature will not change.

CHAnge in **RET**urn temperature (T units) =

Enter the temperature drop for liquid streams returning to the main column, in top-to-bottom order.

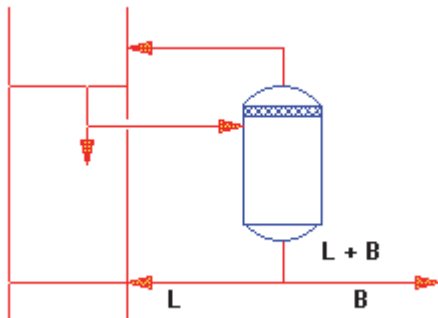
Quick Reference Table of Stripper Specifications

Stripper Type	Number Required	Allowable Specifications X		
		PRO STR	DRA	RET
A. Partial draw, no return	1	X	X	
B. Partial draw, with liquid return	2	X	X	X
C. Total draw, with liquid return required	2	X	X	X

Notes on Specifying Flowrate

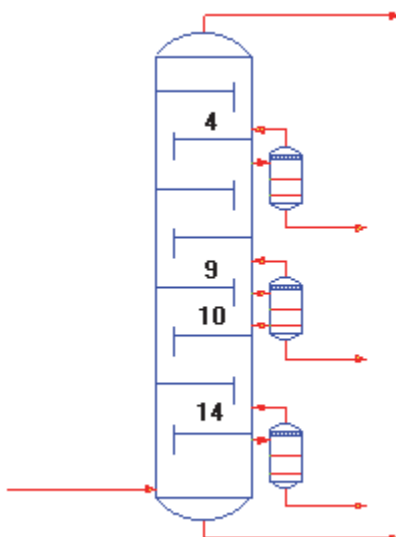
If no liquid is returned from side strippers to the main column, the PROduct from STRipper command overrides any equivalent specification entered with a DRAwrates to strippers command. If liquid is returned, the PRO STR command plus a DRAwrates to strippers command will override any RETurn flowrate command entered.

If you specify RETurn flowrates as less than 1, the value entered is taken as the ratio of liquid returning divided by total liquid leaving the bottom of the stripper $L/(L + B)$ as shown. Do not enter a units option if you are entering fractional values.



If you enter PROducts from STRippers in mass or volume units, you may also enter corresponding molar estimates with the PROduct from STRippers GUEss command to aid the initial program set-up.

Example: Side Stripper Coding



Liquid is drawn from trays 4, 9, and 14 of the main column, and vapor is returned to the trays above the draw trays. The coding for the side strippers is as follows:

```
LOC DRA = 4, 9, 14
LOC VAP = 4, 9, 14
PRO STR (BBL/DAY) = 2100, 3000, 5000
PRO STR GUE = 250, 75, 30
LOC LIQ = 0, 10, 0
RET = 0, 50, 0
```

Refine: Heat Sources

All columns in a rigorous simulation *must* have a heat source at the bottom of the column, even if the amount of heat added is insignificant. For the main column, the heat source can be steam, a reboiler, a heater, or the vapor portion of a feed entering below the bottom tray. For side strippers only steam or reboil are accepted as heat sources. If the column you wish to model has none of these then a dummy heat source must be added with a small duty (e.g. REB (BTU/HR) = 1).

Refine: Steam

If your main column or strippers are steam stripped, you must enter all four of the required steam commands. Steam is handled just like other vapor feeds; it actually mixes on the tray *above* the tray you specify on the LOCAtion of STEam command.

LOCAtion of STEam =

Enter the tray numbers where steam feeds enter the main column and strippers in top-to-bottom order, main column first, then strippers.

NOTE: Steam is a vapor feed; it will mix on the tray above the one you specify. For example, if tray 26 is the bottom main-column tray, you would specify 27 in order to introduce steam below the bottom tray.

PREssure of STEam (P units) =

Enter pressure of all steam feeds in the same order that the feeds are listed on the LOCAtion of STEam command.

TEMperature of STEam (T units) =

Enter temperatures of all steam feeds in the same order that they are listed on the LOCAtion of STEam command.

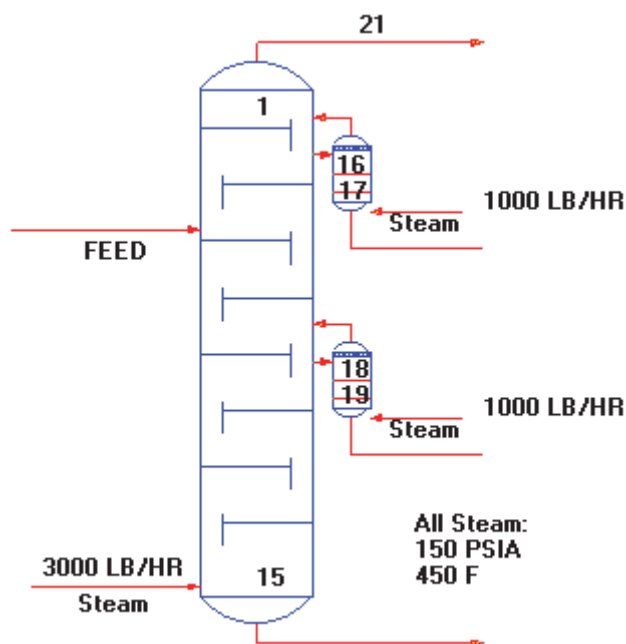
NOTE: DESIGN II checks the phase for steam at the pressure you have specified. If your steam temperature is close to the saturation point, be sure to round up the value to ensure that water will be vapor. Water vapor enthalpies are positive; liquid enthalpies are negative.

STEam rates (Q units/t units) =

Enter the flowrates of all steam feeds in the same order as they are listed on the LOCAtion of STEam command.

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Example 1: Specifying steam

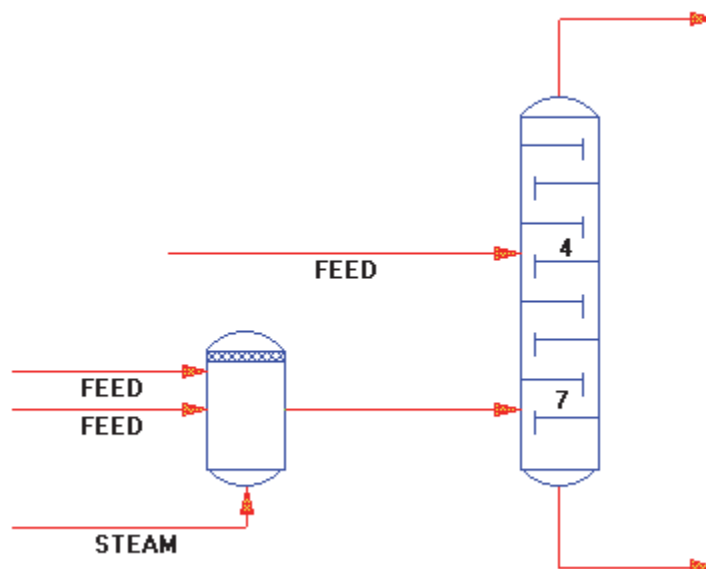


LOC STE = 16, 18, 20, PRE STE = 3*150

TEM STE = 3*450

STE (LB/HR) = 3000, 1000, 1000

Example 2: Mixing steam with a feed



LOC FEE = 4, 7, 7

LOC STE = 8

Alternatively, if you want to see the effect of steam mixing with your hydrocarbon feeds, mix the feeds with a pure water stream (steam) in a MIXer module. Code the outlet stream from the MIXer as the second feed to the REFIne column.

Refine: Reboilers

If your main column or side strippers have reboilers, you must enter reboiler specifications using the following commands. All reboiler commands must include entries for the main column and all side strippers, so that DESIGN II will know where the reboilers are located and which specifications apply to which reboilers. The first entry is always for the main column and is followed by entries for each side stripper in top-to-bottom order. Enter zeroes as position holders when one or more of the columns do not have a reboiler or when a particular specification does not apply to that reboiler.

Identify Reboiler Type

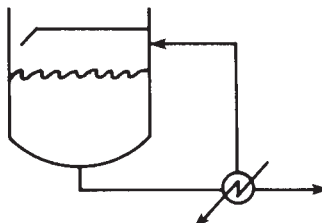
There are two kinds of reboilers available in the REFIne module, kettle and thermosiphon. The thermosiphon reboiler has 3 different configurations. Different types can be combined in a simulation. Assumptions are:

- there is no mixing of return vapor and downcomer liquid
- pump "work" input is zero
- there are no heat losses in the reboiler system

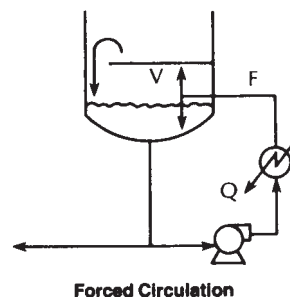
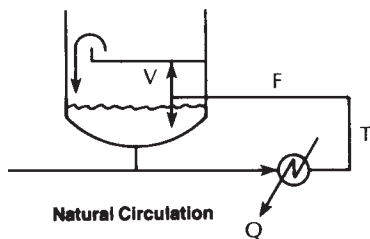
REBoiler TYPE =

Enter reboiler type for the main column first, then for each side-stripper reboiler in top-to-bottom order. If you do not specify reboiler types, REFIne assumes all reboilers to be Type 1.

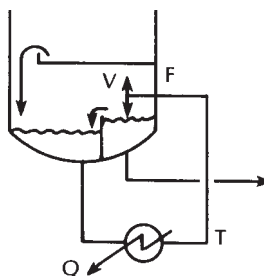
Type 1. Kettle (default)



Type 2. Recirculating (Thermosiphon)

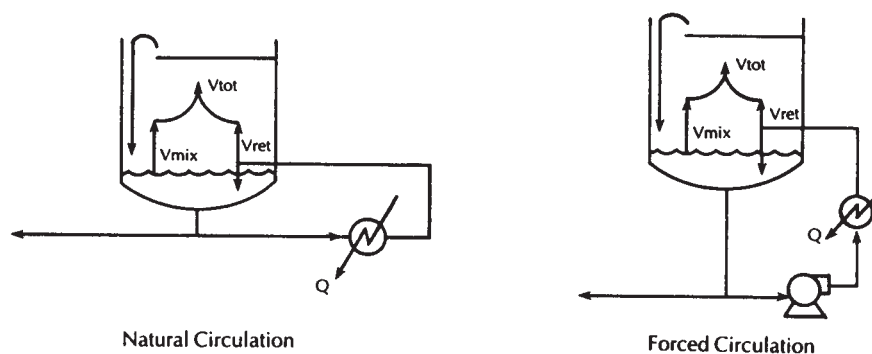


Type 3. Hot Draw Recirculating



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Type 5. Recirculating with Vaporization



The Type 5 has the same reboiler configuration as the type 2 Recirculating Reboiler. However the calculated vaporization rate to the bottom tray (V_{tot}) has been enhanced. The bottom tray downcomer liquid is mixed with the reboiler return liquid and an additional vaporization (V_{mix}) occurs. The V_{mix} rate is added to the reboiler return vapor (V_{ret}) to yield a total vapor rate ($V_{tot} = V_{ret} + V_{mix}$) returned to the bottom tray.

Required Specification for Type 1 Reboilers

The only required command for Type 1 is REBoiler duty.

REBoiler duty (H units/t units)=

Enter duty for the main-column reboiler first, then for each side-stripper reboiler in top-to-bottom order.

Required Specifications for Types 2, 3, and 5 Reboilers

Types 2, 3, 5 require two specification commands from the list below. If more than two commands are entered, DESIGN II will interpret the two commands which are highest in the list as the specifications and the others will be initial guesses. Negative values also indicate initial guesses.

REBoiler EXIt VAPorization percent=

Enter the reboiler return vapor content in weight percent.

REBoiler FLOWrate (Q units/t units) =

Enter inlet liquid flowrate to each reboiler.

REBoiler duty (H units/t units)=

Enter duty for the main-column reboiler first, then for each side-stripper reboiler in top-to-bottom order.

REBoiler TEMperature (absolute T units) =

Enter reboiler outlet temperatures in degrees Rankine or Kelvins separated by commas.

Required Initial Guesses for Types 2, 3, and 5

Reboiler types 2, 3, and 5 require initial guesses for REB FLO and REB duty commands if the commands were not chosen as specifications above. To indicate an initial guess, enter a negative value. Thus every type 2, 3, and 5 reboiler will have a positive or negative value in the REB FLO and REB commands.

REBoiler FLOWrate (Q units/t units) =

Enter a negative value to indicate initial guesses for reboiler feed rates.

REBoiler duty (H units/t units)=

Enter a negative value to indicate an initial guess for duty, main-column reboiler first, then for each side-stripper reboiler in top-to-bottom order.

Optional Reboiler Commands

REBoiler VAPor GUEss (molar Q units/t units) =

Enter an initial guess for reboiler vapor returning to the column (for reboiler types 2, 3, and 5 only).

REBoiler return DELta pressure (P units) =

Enter the pressure difference between the reboiler outlet and the column bottom (for reboiler types 2, 3, and 5 only). If not specified, pressure drop is assumed to be the same as the pressure drop per tray in the column.

REBoiler NAME =

Enter a name for each reboiler with this command (for ALL reboiler types). Each name must be 16 characters or less. The names will appear in the printout.

Special Notes for FIX commands

If you are varying thermosiphon reboiler (REB TYP = 2,3 or 5) duty with a FIX command, then the normal reboiler specification hierarchy changes. The new hierarchy is as follows:

1. FIX command and REBoiler FLOW
2. FIX command and REBoiler TEMperature

3. FIX command and REBoiler EXIt VAPorization

A value must be entered for the REBoiler duty, but it will be adjusted to meet the FIX specification.

Example: Reboiler Coding

For a Type 2 reboiler, the specifications to be entered are reboiler flowrate and weight percent vaporized. Guesses are to be entered for reboiler temperature and reboiler duty.

```
REBoiler TYPE = 2
REBoiler EXIt VAP = 10 REBoiler FLOW = 4200
REBoiler duty = 60E6 REBoiler TEMperature = 350
REBoiler DELta pressure = 2
REBoiler TEMperature (R) = -809.96
```

Refine: Feed Vapor As Column Heat Source

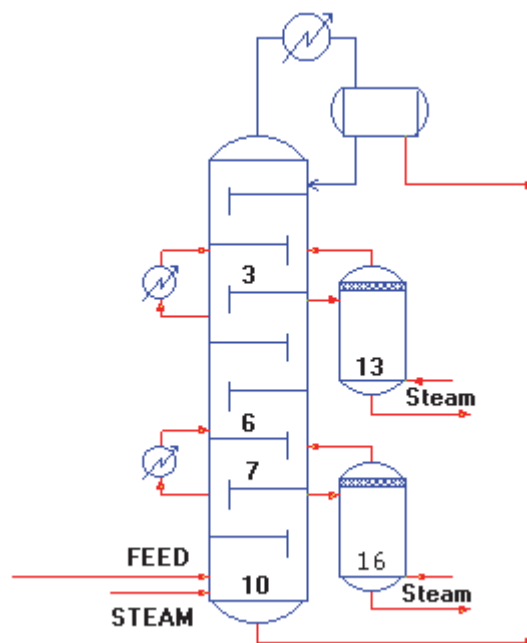
The heat contained in the vapor portion of your feed can also be used as the heat source for the REFIne column. Specify the feed tray location as one tray larger than the main column bottom tray. The vapor feed then enters the column and rises to mix with the tray above the feed tray.

However, when the heat source feed is two-phase, it is desirable to have the whole feed entering the column (not below it) so that you can see any mixing effects between the column liquid and the feed liquid. Entering the feed on the bottom tray would result in the following error message: (NO COLUMN BOTTOMS HEAT SOURCE IS FOUND) and stop the calculation. Therefore, to enter the heat source feed on the bottom tray (instead of below it) you can add a small dummy duty either as reboil or steam to satisfy the program's requirement for a heat source.

Example: Two Phase Feed As Heat Source: Use of dummy REBoiler

```
TOT
STA = 10, 3, 3
LOC FEE = 10
REB (BTU/HR) = 1
LOC STE = 14, 17
STE (LB/HR) = 500, 700
TEM STE = 2*450
PRE STE = 2*150
etc.
```

NOTE: The steam commands refer to the steam feeds for the strippers. The mixing effect on the 2-phase feed is retained and a reboil duty of 1 Btu/hr has a negligible impact on the column



Refine: Heaters and Coolers

You can add heat to or remove heat from any tray using these commands. Both commands must be used.

LOCation of HEATers =

Enter the tray numbers (in top-to-bottom order) on which there are heat additions or removals.

HEAT added or removed (H units/t units) =

Enter the amount of heat added to (positive value) or removed from (negative value) a tray. The entries must be in the same order as the tray numbers listed on the LOCation of HEATers command.

Specifying Heaters and Coolers

1. Do not enter condenser duties with the HEAT command. Condenser duty is specified using the DUTY of condenser command.
2. The enthalpy balance calculated for a tray takes into account all liquids and vapors entering the tray, including liquid portions of feeds on the tray and vapor portions of feeds from the tray below.
3. If you do not know a pumparound rate, you can achieve a similar effect by using the LOCation of HEATers commands and the HEAT commands (enter negative values). This is most useful in initial runs.
4. For columns which expect top-tray pumparounds (PUM REF, PUM TOT, PUM PAR), you can specify the heat removed by the pumparound with the HEAT command. DESIGN II will adjust top and bottom product rates to achieve the value

entered (if no values are entered with a PRO command for top or bottom product. Use the LOCation of HEAters command to specify the correct tray. These commands would replace the need for a top pumparound specification.

Refine: Pumparounds

REFine accepts all commonly found types of pumparounds. Many more systems, not necessarily heat removals, can be modeled also (for example: spray systems, wash sections - where liquid is removed and returned with only nominal heat loss). The number of pumparounds is essentially unlimited and liquid may be withdrawn and returned to almost any tray or mixed with any feed. Pump-ups, pump-downs, and pumparounds are permitted.

Pumparounds can be usefully linked with FIX commands, for example to set minimum liquid runback flows from trays in order to maximize heat removal without drying up a column. Another example might be to set a tray temperature to avoid undesirable events (water condensation, cracking, etc.).

Care should be exercised in simulating existing pumparounds to check precisely where the liquid leaves and re-enters the mass balance, that is, check which active tray areas the liquid flows across. This, combined with the low fractionation efficiency found in heat exchange sections, often leads to over specification of the number of theoretical trays in the pumparound section.

One novel use of pumparounds is to simulate liquid weeping by withdrawing liquid and bypassing the appropriate tray section (specify only nominal heat removal).

The pumparound heat removal can be directly specified or calculated based on return temperature or change in temperature for pumparound liquid. Heat addition is NOT permitted.

Location of Pumparounds - Hydrocarbon or Water

LOCation of PUMparounds =

Enter the draw tray and return tray for each pumparound in top-to-bottom order. First entry is the top-pumparound draw tray; next is its return tray. Third and fourth entries are draw and return trays for the second pumparound, and so on. Enter locations for both hydrocarbon and pure water pumparounds.

A value of -n for a return tray means that the return will mix with the nth feed (in top-to-bottom order) instead of returning directly to the main column.

LOCation of PUMparound for WATER =

Enter value of 1 for pumparounds which are pure water, value of 0 for pumparounds which are hydrocarbon liquids. For each pair of entries on the LOC PUM only one entry (1 or 0) is given here.

Required Pumparound Specifications

Choose **two** of the following commands for each pumparound. Each command used must have entries for all pumparounds, enter a zero for each pumparound for which a specification does not apply. This will maintain the top-to-bottom order.

PROduct of PUMparound (Q units/t units) =

Enter pumparound flowrates for each pumparound in top-to-bottom order. Enter negative values to indicate initial guesses only.

HEAt from PUMparounds (H units/ t units) =

Enter the amount of heat removed from pumparounds in top-to-bottom order.

TEMperature of PUMparounds (T units) =

Enter the temperature of pumparound returns, in top-to-bottom order. If you specify a temperature higher than the bubble-point temperature, no heating will occur, and return temperature will not change.

CHANGe of PUMparound temperature (T units) =

Enter the temperature drop for pumparounds in top-to-bottom order.

Optional Molar Flowrate Guesses

PROduct PUMparound GUEss (molar Q units/t units) =

If you enter pumparound rates in mass or volume units, guesses for the molar equivalent of those rates are required. You do not have to provide composition guesses.

Notes on Specifications

1. Each pumparound on a main column must have two specifications in addition to the LOC PUM command. You do not have to use the same specifications for all of the pumparounds. Each specification command, however, must have an entry for all pumparounds in top-to-bottom order. Enter a zero for any pumparound to which the command does not apply. For example, if a column has three pumparounds and all four specification commands are used, the entries could look like the following:

```
PRO PUM=X, 0, 0
HEA PUM=0, X, X
CHA PUM=0, X, 0
TEM PUM=X, 0, X
```

The X's represent nonzero entries. Note that the top, middle and bottom pumparounds all have two specifications.

2. A combination of PROduct of PUMparound and HEAt from PUMparound is the easiest to converge, while the combination of TEMperature of PUMparound and CHANGe of PUMparound temperatures for a pumparound is the hardest to converge.

3. A CHAnge of PUMparound temperature greater than 200F is frequently difficult to converge.
4. The REFine module will calculate the required pumparound rate if you specify two of the following three commands:

```
HEAT from PUMparound
TEMperature of PUMparound
CHAnge of PUMparound temperature
```

If you do this, you should enter an estimate for the pumparound rate by specifying a negative value on the PROduct of PUMparound command. See Example 1 below.

Example 1: Pumparounds with Flowrate Guesses

```
LOC PUM = 5, 5, 7, 8, 13, 10
HEA PUM = 10E6, 35E6, 40E6
TEM PUM = 0, 350, 0
CHA PUM = 0, 0, 150
PRO PUM = 750, -1000, -1000
```

Example 2: Water Pumparounds

For quench columns, one or more of the pumparounds is pure water.

The coding is handled in the following manner:

```
STA = 12
LOC PUM = 3, 1, 3, 2, 8, 5, 9, 9
LOC PUM WAT = 1, 1, 0, 0
PRO PUM = 15000, 33000, 1500, 1650
HEA PUM = 120E6, 225E6, 50E6, 75E6
```

The LOCation of PUMparound WATER command indicates that the first and second pumparounds specified on the LOCation of PUMparound command are pure water, the third and fourth pumparounds are hydrocarbon liquids.

Refine: Fix Tray Conditions

The FIX commands are useful for the user to control certain internal column parameters which would otherwise float. In this manner a simulation can be directed to converge in a constrained manner to fulfill a specified objective.

You can use several FIX commands in any REFine module to set the temperature, liquid rate, or vapor rate for selected trays. For each FIX command, you must also select a duty or product rate that can be varied in order to satisfy the parameter being fixed.

Some of the more common applications for FIX commands are to:

- set the overflash
- set the runback from a stripper draw tray
- set the reflux rate
- set the top tray temperature for internally refluxed columns
- set the flash zone temperature
- set vapor rate returning from a reboiled side stripper

The application of FIXes is useful for both building an initial column model (for example to set the overflash rate by varying the feed heater to avoid insufficient heat input) and for fine tuning a final column model (for example to set a tray condition precisely).

FIX Command Format

All FIX commands are entered in the following format:

Command format	FIX parameter (units) i = value, tray, variable
Example commands	FIX TEM (C) 1 = 110, 1, 1 FIX LIQ NET (BBL/DAY) 2 = 500, 20, H1 FIX TEM 3 = 670, 22, P5

where:

parameter can be	LIQ uid rate from a tray LIQ uid NET rate from a tray (rate to the next lower tray after subtracting all liquid draws) VAP or rate from a tray TEM perature of a tray
units	refers to the input units of the specified value. Defaults are LBMOL/HR for liquid and vapor rates, and F for temperatures. Other common units such as BBL/DAY must be entered here in parentheses.
i (from 1 to n.)	Each FIX command must be labeled with a sequential number that follows the top-to-bottom convention, 1 for the first FIX command affecting the highest tray, 2 for the second highest FIX command, and so on.
Value	is the desired value of the fixed parameter.
Tray	is the tray number of the quantity being fixed. Caution: define the <i>tray</i> number, not the stage number. Example: the topmost tray would be defined as tray 1 even though it may be stage 2 if the condenser is counted as an equilibrium stage. The condenser is numbered as tray zero.

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variable can be: a duty on a tray, enter tray number; a feed heater, enter **H** and a feed number; or a product flowrate, enter **P** and a product number

If the variable is a number, then it is the **tray** location of a duty that will be varied, i.e., a heater duty, condenser duty, reboiler duty, or pumparound duty. When controlling pumparounds, you should enter the tray number of the pumparound *return*.

If the variable is entered as a number preceded by the letter "**H**", then it is the number of a feed (top-to-bottom order) **furnace**. DESIGN II will vary the furnace duty for that feed, thereby adjusting the inlet temperature to the column (outlet temperature from the furnace).

NOTE: This is the feed number in top-to-bottom order, not the stream number.

If the variable is entered as a number preceded by the letter "**P**", then the number is the **product** (in-top-to-bottom order) whose rate will be varied. The top-to-bottom order is based on draw location; side stripper products are numbered before the bottom product. If a tray has both unstripped and stripped product draws, the unstripped product is numbered first.

Optional Molar Flowrate Guesses

FIX GUEss (molar Q units/t units) =

Enter molar flowrate guesses if one or more FIX commands are given in mass or volume units. Enter values in top-to-bottom order, separated by commas.

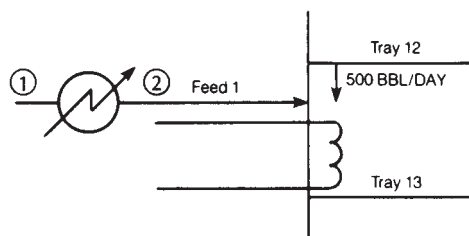
General Rules for FIX Commands

1. The quantity being fixed must be something that would otherwise float in the absence of a FIX command.
2. The quantity being varied must be something that would otherwise be specified in the absence of the FIX command. So if a pumparound duty is to be varied with a FIX, the pumparound must have a HEAT from PUMparound specification. Similarly if the bottom product flowrate is to be varied with a FIX, its flowrate must be specified with the PROduct rate command.
3. A duty that is varied must be at or below the location of the quantity being fixed.
4. Product rates cannot be fixed (use PRO or PRO STR instead).
5. There can only be one FIX command on any tray.
6. There can only be one duty varied on any tray.
7. At least one stage must remain free of FIX commands or other commands that affect the heat balance or material balance (for example, TEM CON=).
8. FIX commands are numbered sequentially from top to bottom of the column.
1. If liquid or vapor rates are specified in mass or volume units, you should enter a FIX GUEss command to supply molar guesses for each FIX LIQ, FIX LIQ NET and FIX VAP in top-to-bottom order. All values for guesses are entered on one FIX GUEss command.

Example 1: Setting the Overflash

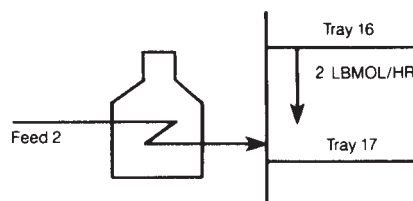
a. by varying a heater duty on feed tray 13

```
HEA EXC 1 = BUB, 1,-2,TEM OUT BUB
REFI 2 = STAB, 2,-3,-4,-5,
FIX LIQ (BBL/DAY) 1 = 500,12,13 FIX GUE = 2
LOC FEE = 13, LOCHEA = 13, HEA (BTU/HR) = 30E6
```



b. by varying the feed furnace heat on feed 2 entering tray 16.

```
FIX LIQ (BBL/DAY) 1 = 500,16,H2
FIX GUE = 2
LOC FEE = 5,17
```



A feed furnace can only be varied to set the liquid rate of the tray *immediately* above that feed tray (17 is the feed tray location of Feed 2).

The FIX LIQUid command sets the rate of all liquid leaving a tray, including any unstripped draws, draws to side strippers, and draws to pumparounds. Options a and b will have different output. When a furnace duty is varied, the feed flash result is given for the conditions entering the tower, after the furnace. When a tray duty is varied, the flash result given is at the conditions before the heat addition. Therefore, the actual feed temperature must be calculated by the user from the tray duty and the results of a HEATING CURve. When option a is used, the feed should enter at its bubble point. It may be necessary to put a HEAT EXChanger module with a TEM OUT BUB spec in front of the column. This ensures that all of the feed is exposed to the heat source. Option a should be used whenever the feed temperature must be raised more than 150-200 F, to ensure

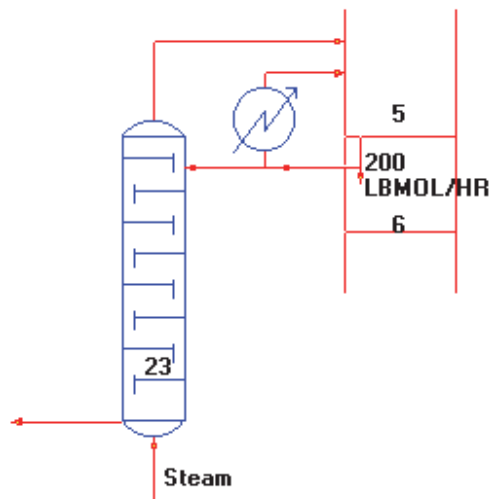
convergence.

NOTE: Feed furnaces cannot cool. Do not start calculations with a feed temperature which is very close to the expected furnace exit temperature.

Example 2: Setting Runback from a Stripper Draw Tray

```
FIX LIQ NET1=200,5,5
LOC PUM=5,5
PRO PUM=1000
HEA PUM=10E6
LOC DRA=5
PRO STR=250
```

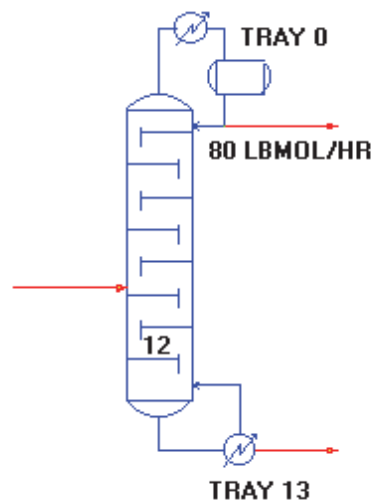
The FIX LIQ NET command sets the net liquid rate falling to the tray below after accounting for all liquid draws. For this case, you would set the pumparound rate with a PRO PUM command and provide an initial guess for the pumparound duty with a HEA PUM command.



Example 3: Setting Reflux Rate

```
FIX LIQ NET 1=80,0,13
REB=5E6
STA=13
TOT
```

The FIX LIQ NET command is used to set the reflux rate (the liquid returning to tray 1 from tray 0) for a reboiled column by varying the reboiler duty. The value on the REBoiler duty command will be used as an initial guess.



Example 4: Setting Top Tray Temperature for Internally Refluxed Columns

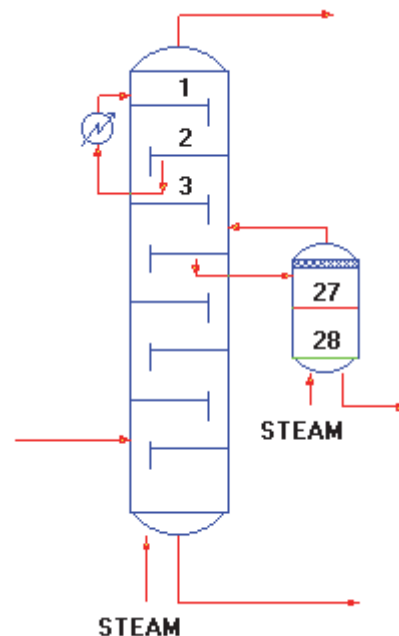
For the PUM REF, PUM TOT, and PUM PAR configurations which are not externally refluxed, the FIX TEM command is available for setting the temperature of the top tray, i.e., the temperature of the internal condenser.

```
FIX TEM(C) 1=110, 1, 1
LOC PUM=2, 1
PRO PUM=250
HEA PUM=14E6
PRE TOP (MMHG) =50
PUM REF
```

For this case you would usually specify the PUM REF configuration, indicate the pumparound draw and return trays (LOC PUM=2,1), set the pumparound rate with the PRO PUM command, and provide an initial guess for the pumparound duty with the HEA PUM command. DESIGN II will adjust the duty on tray 1, i.e., the pumparound duty. The top and bottom product rates from the column are also adjusted to meet the temperature specifications.

Be sure to check the steam tables to ensure that water is a vapor at the temperature and pressure conditions you are establishing for the top of the tower.

When using FIX TEM to set the temperature for the top tray, the TEM TOP guess should be the temperature for tray 2.



Example 5: Setting Flash Zone Temperature

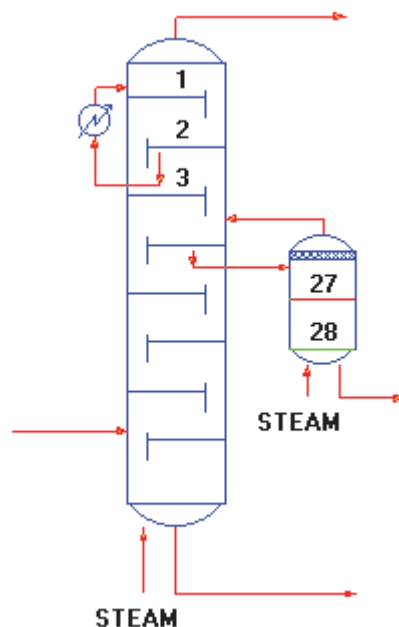
This FIX TEM command is not typically used unless a converged run gives a flash zone temperature unacceptably higher or lower than preferred. In such cases, prudent application of the FIX TEM command will adjust the flash zone temperature accordingly. General rules for the FIX TEM command follow.

- If the flash zone is too hot, vary a product rate below the flash zone.

```
FIX TEM1=670, 22, P6
PRO =0, 0, 250
```

Increasing the bottom stream flowrate will withdraw more heavy components (with higher boiling points) thus lightening the composition and lowering the equilibrium temperature on trays above the bottom draw.

In the above example where the bottom product rate is being varied, the bottom product rate *must* be specified with the PROduct rate command.

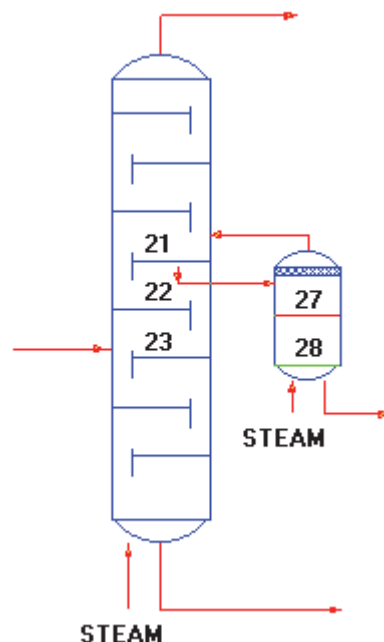


- b. If the flash zone is too cold, vary a product rate above the flash zone.

FIX TEM1=670, 22, P5
PRO =10, 150, 0

Increasing a draw rate above the feed tray will increase the amount of heavy components (with higher boiling points) thus going past the equilibrium temperature. To allow material to move from the bottom of the column instead of the top, specify the overhead product rate on the PROduct rate command (thus allowing the bottom rate to float).

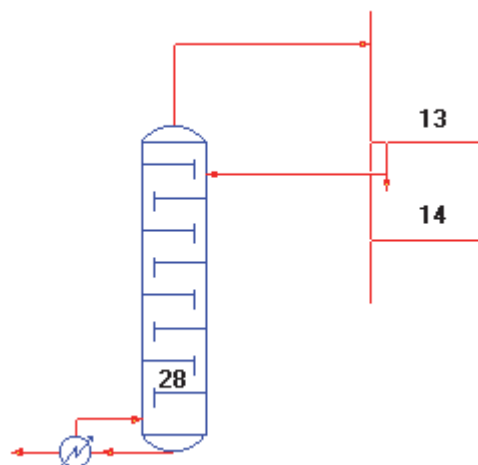
If the flash zone temperature is too cold and you decide to use a FIX TEM command, you **must also** either increase the feed temperature or add a FIX LIQ command which will set the overflash by varying the feed furnace to increase the feed temperature. Remember to number your fixes in top-to-bottom order.



Example 6: Setting Vapor Rate Returning from a Reboiled Strippper

STA = 22, 7
FIX VAP1=70, 0, 29
REB=0, 5E6

The FIX VAP command is rarely used with one exception - specifying the vapor return from a reboiled stripper rather than specifying the reboiler duty for the stripper. In this case, you enter a *zero* for the stripper tray from which the vapor is leaving, *not* the tray number. This tells DESIGN II that the vapor whose rate you intend to fix is returning to the main tower from the stripper. You would also supply an initial guess for the reboiler duty with the REB command.



Refine: Internal Stream Commands

Internal streams are very useful when it is required to view the results of a stream that are internal to the REfine Column, after a column has been converged. The details of streams going in and out of column components such as condenser, reboiler, side-stripper, pumparound, side heater or cooler is easily obtained by using these commands. Information on temperature, pressure, and flow of each component or cuts are accessed and is displayed in the stream summary and detailed stream summary sections. Note that the numbers used for these streams should not be on the flowsheet except for those specified as products or sidedraws. Specific internal stream commands are listed below.

Condenser Internal Streams

INT CON STR = x, -y

Enter this command for columns with condensers, where x is a stream number assigned to the tray 1 vapor and y is a stream number assigned to the product to the reflux accumulator.

INT CON SEP = x, -y

Enter this command for columns with condensers, where x is a stream number assigned for the vapor leaving tray 1 at the condenser outlet conditions and stream number 'y' is assigned to the stream refluxed back to the main column excluding any liquid distillate and decanted water.

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INT CON DEC = x,

Enter this command for columns with condensers having decant, where x is a stream number assigned for the decant.

Reboiler Internal Streams

INT REB STR = x, -y,

Enter this command for columns with reboilers, where x is a stream number assigned to the reboiler feed and y is a stream number assigned to the reboiler return.

Side heater Internal Streams

INT HEA STR INO = x, -y

Enter this command for columns with side heaters. 'INO' represents the draw tray number for heaters or coolers. x is a stream number assigned to the side-heater/cooler feed, and y is a stream number assigned to the side-heater/cooler return.

INT FEE HEA INO = x,

Enter this command for columns with side heaters. 'INO' represents the draw tray number for heaters or coolers. x is a stream number assigned to the side-heater/cooler return.

Pumparound Internal Streams

INT PUM STR INO = x, -y

Enter this command for any column with pumparounds where 'INO' represents the draw tray number for pumparounds. x is a stream number assigned to the pumparound feed, and y is a stream number assigned to the pumparound return.

Side-Stripper Internal Streams

INT STR STR INO = x, -y (OR)

INT STR STR INO = x, -y, -z

Enter this command for any column with side-stripper where 'INO' represents the draw tray number for side strippers. x is a stream number assigned to the side-stripper feed, y is a stream number assigned to the side-stripper return and z is a stream number assigned of stripper has liquid return

INT STR REB INO = x, -y

Enter this command for any column with side-stripper with reboiler where 'INO' represents the draw tray number for side strippers. x is a stream number assigned to the side-stripper's reboiler feed, and y is a stream number assigned to the side-stripper's reboiler return.

NOTE:

1. INO is the draw tray number for pumparounds, side strippers and heaters/coolers.
2. STR stands for stream (not required, except for STRipper).
3. DEC is only for condenser decant.
4. The stream numbers used for internal streams should not be connected to other external process equipment modules. You can use the Inline FORTRAN COPSTR (i, j) function to copy the stream composition to another stream for additional calculations. See Inline Fortran: Table 5. Utilities Subroutines (use with CALL) for more details.

Refine: Product Property Specifications

Use the PROduct SPECification command to specify a product "quality" by varying a product flowrate. The product you choose to vary *must* be a specification on the PROduct rate or PROduct STRipper commands. Using the PRO SPE command can eliminate the need to make numerous trial and error runs.

The PRO SPE command is int

units	refers to the input units of the specified value
j	is a number from 1 to n, each PRO SPEC must be numbered in top-to-bottom order based on draw location.
value	is the desired value of the property specified property is one of the product quality specifications, such as ASTM IBP , listed in Property Keyword Table below
product	is PRODn where n is the product number (in top-to-bottom order) of the product to which the specification applies (based on product draw tray order)
variable	is PRODn where n is the product number (in top-to-bottom order) of the product whose rate will be varied to meet the specification

Property Keyword Table

ASTM IBP	D-86 initial boiling point (*)
ASTM 5PT	D-86 5% point
ASTM 95PT	D-86 95% point
ASTM 98PT	D-86 98% point
ASTM EP	D-86 end point (*)
ASTM GAP	D-86 5% point of the next heavier product minus the 95% point of the specified product
TBP IBP	TBP initial boiling point (*)
TBP 5PT	TBP 5% point
TBP 95PT	TBP 95% point
TBP EP	TBP end point (*)
PUR COM n	mole fraction of the nth component in the COMponent list
PUR COM n TO m	total mole fraction of the nth to mth components in the COMponents list.
AMW	average molecular weight
GRA	average gravity
FLA	flash point
FLO	mass or volume ended for tuning up product property specifications by making moderate adjustments in product rates (approximately 10%).

Before using it, you should have achieved a ballpark solution by changing the number of stages, feed and draw locations, and duties. Do not use the PRO SPE command until you have converged results. Then add your PRO SPE commands, update your temperature and molar flowrate guesses, and rerun the simulation.

PROduct SPECification Format

Specify a product property by varying a product. Enter one PRO SPE command for each product specified.

Command format

PRO SPE (units) j= value, property, product, variable

Example commands

PRO SPE (F) 1 = 550, ASTM95PT, PROD3, PROD4

PRO SPE (F) 2 = 760, ASTM95PT, PROD4, PROD5

where: flow rate (*must* specify mass or volume units for this option)

VIS SET n viscosity from the nth viscosity data set

PRO SET n user entered property from the nth user entered property data set

POUR pour point from the user entered pour point data

You may specify viscosity, pour point, or other properties if you have entered the appropriate data using the feed viscosity and property commands.

* The default value for initial boiling point is 2 volume percent; default for end point is 98 volume percent. These values can be changed using the PRO IBP and PRO EP commands respectively. Typical IBP values are 0, 1 or 2; typical EP values are 98, 99 or 100.

Making Feasible Specifications

It is, of course, essential that the quality specifications are reasonable and feasible. The following may provide help in achieving this:

1. ASTM gaps are primarily controlled by the number of stages in the column, the amount of reflux, the amount of overflash, and the amount of stripping steam. You should not expect to alter the gap substantially with the PRO SPE command, which only varies product rates.
2. Do not attempt to specify the IBP or 5% point of the lightest product, or the EP or 95% point of the heaviest product. They are controlled by the IBP and EP of the feed stream, not by the column product rates.
3. Be sure PURity specs are consistent with the overall material balance. The mole fraction specified times the flow of that product must not be more than the amount of that component in the feed.
4. In most cases, it is not reasonable to make more than one specification on a given product. For instance, if you specify the gravity of a particular product, you should not also specify its molecular weight.
5. If meeting your specification requires varying the product rates by more than about 10%, the column may not converge. You should try to get your initial solution closer to spec before adding the PRO SPE command.

Choosing Which Product Rate to Vary

Several principles are involved in deciding which product rate to vary in order to meet your specification. First, the product rate being varied *must* be one that would be a specification if the PRO SPE command were omitted. This means that a value for the product rate to be varied must be entered on the PRO or PRO STR command as though it were a specification. This value

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will be used as an initial guess. Also, the same product rate may not be varied by more than one PRO SPE command.

Finally, the most important principle in choosing which product rate to vary is that it must in some way be directly related to the property you wish to specify. That is, you should be able to find a direct mechanism by which a change in the chosen product rate will produce a measurable change in the specified property (but not adversely affecting adjacent streams).

Example 1: Achieve a 550 F ASTM 95% point on product 3 by adjusting the rate of product 4, and a 760 F ASTM 95% point on product 4 by adjusting the rate of product 5.

```
PRO SPE1 = 550, ASTM95, PROD3, PROD4
PRO SPE2 = 760, ASTM95, PROD4, PROD5
```

Example 2: Specify a viscosity of 1.6 centipoise at 100 F for the fifth product by varying the sixth product. (Feed viscosity data at 100 F were entered as FEE VIS SET 1)

```
PRO SPE1 = 1.6, VISSET1, PROD5, PROD6
```

Example 3: Specify an API gravity of 19 for the bottoms product

```
PRO SPE1 = 19, GRA, PROD5, PROD5 PRO= 0,880
PRO STR = 580,230,470
```

Explanation: Varying the bottoms product rate will produce a measurable change in the gravity of the bottoms product because as the rate changes, lighter material will be shifted from the next lighter product into the bottoms, or vice versa. The bottoms rate of 880 lbmol/hr, which would be used as a specification if the PRO SPE command were omitted, will be used as an initial guess. The stripper rates will be used as specifications.

Example 4: Specify a 225C ASTM 95% point on product 2. The distillate product rate is a specification also.

```
PRO SPE(C) 1 = 225,ASTM 95PT,PROD2, PROD2 PRO (KG/HR) = 2500,0
PRO STR (KG/HR) = 10000,12000
```

Explanation: In order to achieve the ASTM 95% point of product 2, material must be exchanged with product 3. Since the rate of product 1, the distillate rate, is fixed, the light end of product 2 is fixed also. Therefore, if we want to shift the heavy end of product 2, we must change its flowrate. The product 2 flowrate, which would ordinarily be specified, is therefore allowed to vary. The 10000 kg/hr value will be used as an initial guess.

Example 5: Specify a 225 C ASTM 95% point on product 2. The bottoms product rate is a specification also.

```
PRO SPE(C)1 = 225,ASTM 95PT, PROD2, PROD3 PRO (KG/HR) = 0,30000
PRO STR (KG/HR) = 10000,12000
```

Explanation: Again, as in Example 2, in order to affect the ASTM 95% point of product 2, material must be exchanged with product 3. In this case, however, the bottoms rate (product 4) is fixed. If the rate of product 3 were also fixed, then that would fix the heavy end of product 2. Thus no material could be exchanged between product 2 and product 3. Therefore, the rate of product 3 must be varied to achieve the ASTM 95% point spec on product 2. The value 12000 kg/hr will be used as an initial guess for product 3.

Example 6: Specify a distillate product rate of 2000 bbl/day and a bottoms product rate of 4500 bbl/day. The flash point of the heavier of two unstripped draws should be 180FF.

```
PRO (BBL/DAY) = 0,3000,1500,4500
PRO SPE (BBL/DAY) 1 = 2000,FLO, PROD1,PROD2
PRO SPE 2 = 180,FLA,PROD3,PROD3
```

Explanation: Ordinarily, you must specify the rates of all unstripped draws, and you may specify either the distillate or the bottoms rate, but not both. The PROduct command shown here, if entered alone, would set the two draw rates and the bottoms rate. The first PRO SPE command sets the distillate rate by allowing the first side draw rate to vary. Now that we have specified both the distillate rate and the bottoms rate, we know that the flowrates of the two side draws must add up to a constant amount to satisfy the mass balance. To control the flash point of the heavier draw, material must be exchanged between the two draw products. Therefore, the flowrate of both must vary because the two together have a fixed total flow. Since the lighter draw is already varying, the second PRO SPE command must allow the heavier draw to vary. In this situation, the 3000 and 1500 bbl/day rates entered on the PRO command for the two draws will be used as initial guesses.

Refine: Tray Sizing

There are two different short-cut sizing techniques in the REFine column calculations. Both calculations are performed automatically using default values unless you enter one or more of the commands listed below.

Smith-Dresser-Ohlswager Technique

The first is the Smith-Dresser-Ohlswager technique (Smith, R.B., Dresser, T. and Ohlswager, T., *Hydrocarbon Processing*, Vol. 40, No. 5., pp. 183- 184 (1963)). This correlation calculates the column diameter at 100 percent of flood.

The method is generally applicable to bubble cap, sieve and valve trays and can be subject to considerable error. It should not be used for final column design. The correlation has limits for the liquid to vapor ratio and warning messages indicate when the limits are exceeded.

All commands are optional. If you do not want to use the default 18 inches settling height, you must enter all of the following commands:

SPAcing of TRAYs (L units)=

Enter the tray spacing to be used along with WEIr HEIght and WEIr LENgth in calculating the settling height. Default is 18 inches settling height.

WEIr HEIght (L units) =

Enter the WEIr HEIght to be used along with SPAcing of TRAYs and WEIr LENgth in calculating the settling height.

WEIr LENgth (L units) =

Enter the WEIr LENgth to be used along with SPAcing of TRAYs and WEIr HEIght in calculating the settling height.

DOWncomer AREa (L2 units) =

Enter the downcomer area in square feet. Default is 12 percent of the empty column area.

Values entered with the SPAcing of TRAY, WEIr HEIght, and WEIr LENgth commands are used in calculating the settling height (tray spacing minus clear liquid depth). If any one of these three commands is not entered, the settling height is assumed to be 18 inches. Minimum settling height is 2 inches and maximum is 30 inches for the correlation.

DOWncomer AREa is used in calculating the vapor velocity on each stage. If not entered, this value is set to 12 percent of the empty column area.

Glitsch Technique

The second sizing technique is provided in cooperation with Glitsch Incorporated (Glitsch Bulletin 4900, *Design Procedure for Ballast Trays*). This short-cut method was developed for ballast trays but is also applicable for sieve trays with 14% hole area. This technique is applicable for tray spacings of 12-48 inches and percent of flood values from 20-100%.

By default, the Glitsch, Inc. correlation calculates column tray diameters at 70% - 80% of flood based on tray loadings, system factor and tray spacing. The number of passes will be calculated if you do not specify a value. You can specify a different percent of flood with the GLitsch PERcent flood command.

Optionally, specify the GLitsch DIAMeter and the percent of flood will be calculated. Do not specify both GLitsch DIAMeter and GLitsch PERcent of flood.

GLitsch SYStem factor =

Enter the system factor for foaming on the trays. Default is 1.0 which is appropriate for non-foaming, regular systems. One input value allowed.

GLitsch PERcent flood =

Enter the percent of flood for the column. If not specified, the program will calculate. One input value allowed.

GLitsch PASses per tray per section =

Enter the number of tray passes. If not specified, the program will calculate. One input value allowed: 1, 2, or 4 passes. In REFine columns only, GLitsch PASses can be different and should correspond to the number of GLitsch SWAge trays plus one..

GLitsch SPAcing per tray per section (L units) =

Enter the spacing(s) of trays. Default is 2 feet. The technique is valid for tray spacings from 1 to 4 feet. See GLitsch SWAge command for additional capability.

GLitsch DIAMeter per tray per section (L units) =

Enter the column diameter(s). If not specified, the program will calculate. You cannot specify both GLI DIA and GLI PER. See GLitsch SWAge command for additional capabilities.

GLitsch SWAge trays =

Enter the tray numbers immediately below the swage in the column. The GLitsch SWAge command can be used in conjunction with either GLitsch DIAMeter or GLitsch SPAcing of trays or both for columns with more than one diameter or tray spacing. The GLitsch SWAge command will have one less value than the GLI DIA or GLI SPA commands.

GLitsch DOWncomer AREa per tray per section (L2 units) =

Enter the total downcomer area per tray. Will be calculated, when not provided.

GLitsch WEIr HEIght per tray per section (L units)=

Enter the WEIr HEIght to be used along with GLitsch SPAcing in calculating the settling height. Default is 3 inch.

GLitsch VALve TYPE = 1 or 4

Enter the valve type. Either 1 or 4 is available. Default is 1.

V-1 A general purpose standard size unit, used in all services. The legs are formed integrally with the valve for deck thicknesses up to 3/8"

V-4 This signifies a venturi-shaped orifice opening in the tray floor which is designed to reduce substantially parasitic pressure drop at the entry and reversal areas. A standard ballast unit is used in this opening, normally, although a V-2 or V-3 unit can be used for special services. The maximum deck thickness permissible with this opening is 10 gage.

GLitsch VALve MATerial =

Enter the valve material. Default is carbon steel.

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Material (Keyword in bold)

ALUMinum

CARBon steel (default)

COPPer

MONEl

NICKel 200

HASTalloy

STAINless steel 304

LEAD

TITANium

GLITSch VALve THICKness (L units) =

Enter the valve thickness. Default is 0.06 inch.

GLITSch VALve NUMber (1/L2 units)=

Enter the number of valves per square foot. Default is 13.

GLITSch DECK thickness (L units) =

Enter the deck thickness. Default is 0.104 inch.

It is important to use the correct system factor (GLI SYS=) for foaming on the trays. The default value used by the program is 1.00, which is appropriate for non-foaming, regular systems. Other recommended values for GLITSch SYStem factor are as follows:

System	Value
Lean oil absorbers, amine & glycol regenerators (moderate foaming)	0.85
Amine & glycol contactors (heavy foaming)	0.73
MEK units (severe foaming)	0.60
Caustic regenerators (foam-stable)	0.30

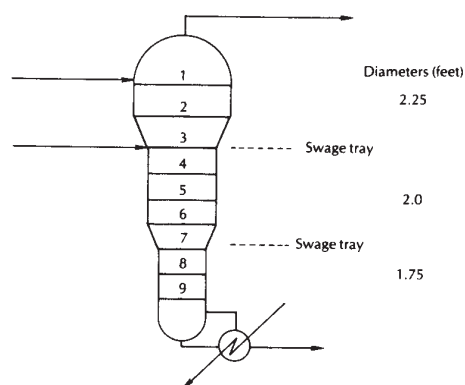
The GLI SYS, GLI PER and GLI PASSes commands are limited to one value per distillation column. The GLITSch SPACING, GLI DIAMeter and GLI PASSes (refine only) commands are allowed multiple values. Use the GLITSch SWAge command to tell the program where the different diameter/spacing sections begin. Values are entered in top-to-bottom order.

Example: Multiple diameters

GLITSch SWAge = 12, 15

GLITSch DIAMeter = 10,2.5,3

GLITSch PASSes = 1, 2, 2 (for Refine column only)



Refine: Calculation Options

Fenske Shortcut Material Balance

FENSke calculation

Enter this command to perform a "Fenske" shortcut material balance calculation only; NOT the rigorous tray-by-tray calculation.

The FENSke calculation command can be inserted anywhere in the keyword commands for the REFine module. When this command is used, the rigorous column calculation is not executed. Instead, DESIGN II checks your input file and performs a fractionation based on the number of stages (material balance only). This command CANNOT be used when either DUTy of CONDenser and REFLux ratio or TEMperature of CONDenser and REFLux ratio are specified.

If you are unsure about the product splits, it is a good idea to make an initial run with the FENSke calculation command. The results allow you to review the product slate quickly and make any adjustments before your rigorous run.

In addition, the shortened printout gives you estimated product rates (in molar units) which can be used as PROduct rate GUESses and PROduct from STRipper rate GUESses for your full rigorous simulation.

Thermodynamics Commands

These commands specify thermodynamic options for the module only when they are different than the system thermodynamics specified in the GENeral section. Options are given in Thermodynamics Section.

HKEy=

Enter symbolic name of enthalpy option. (e.g. **HKE = COPE**)

KKEy=

Enter symbolic name of K-value option. (e.g. **KKE = KVAL**)

DKEy=

Enter symbolic name of density option. (e.g. **DKE = STDD**)

IMMiscible=

Enter the component ID number of the immiscible component. If the K-value does not automatically treat water as immiscible and immiscible treatment is desired, enter IMM = 62. When decanting water, it is recommended to treat water as immiscible. See Thermodynamics Section for immiscible component guidelines.

NO IMMiscible

Enter this command to have water treated miscibly for K-value options which normally treat water immiscibly. Not allowed when decanting water. See Thermodynamics Section. This option is not normally used with Refine columns; not allowed for columns with steam stripping.

Refine: Print Options

Tray Sizing Calculation and Print Options

Choose *one* of the following commands to select which sizing correlation output you wish, if any:

SMIth SIZing OFF

Enter this command to delete the Smith-Dresser-Ohlswager calculation and output.

GLItsch SIZing OFF

Enter this command to delete the Glitsch sizing calculation and output.

COLumn SIZing OFF

Enter this command if no column sizing output is desired in the program output.

Control Column Output

The reports generated by REFIne contain a large amount of information which you may wish to suppress. The following commands permit deletion of whole sections of the output BUT the user is cautioned to be judicious in deletions in case valuable information is lost without knowledge of loss.

REPOrts =

Enter this command to suppress various sections of the rigorous column printout. If it is not used, all possible output (excluding diagnostic information) will be printed. Enter six numerals separated by commas. Enter a zero to obtain printout or a 1 to suppress printout as outlined below. Default set of report options is REP=0,0,0,0,0,0, except for intermediate recycle loop iterations for which the default is REP=1,0,1,1,0,1. We recommend that you NEVER delete the fifth report. The values for the third, fourth, and sixth entries also affect PET STR output.

first entry	= 1	deletes tray-by-tray compositions and K-values plus side stripper vapor return compositions
second entry	= 1	deletes feed flash summary
third entry	= 1	deletes component and cumulative volume percents and laboratory distillations from the product summary
fourth entry	= 1	deletes component gravities, mole, mass and volume amounts from the product summary
fifth entry	= 1	deletes property, temperature, vapor, and liquid profiles
sixth entry	= 1	deletes API viscosities

Example: REP = 1,1,1,1,0,1

Additional Print Control

CONDensing CURve

Enter this command to obtain a condensing curve for the vapor leaving the top tray of the main column. The curve provides information on the gas, two-liquid phase regions (water and hydrocarbon), and the single liquid phase region and is useful for sizing heat exchangers.

PLOT OFF

Enter this command to suppress the graphs of TBP and ASTM curves for products. This does not suppress the tables of TBP and ASTM data for products.

SWItch =

DESIGN II automatically prints column convergence information consisting of the normalized square error in all heat and material balances. The default is SWI= 1. If you enter a 2, you will get extra diagnostic printout containing heat and material balance errors for each stage plus current values of unknowns for each iteration.

PROduct NAMES =

Enter all product names in order from the lightest product to the heaviest. Do not skip any products. Names can be up to

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16 characters long. All names *must* fit on one line; no continuation line is allowed for the PRO NAM command. Do not use DESIGN II input keywords, such as "FLA" in your names. If you do not enter product names, DESIGN II will identify the products in the printout by their draw tray location.

Example: PRO NAM=VENT GAS,LT NAPHTHA,HVY NAPHTHA,KERO,LGO,RESID

Product Cooling Curves

You can request cooling curves to be printed for one or more products and optionally specify the temperature and pressure ranges for each curve with these commands. Only PRO CUR is required for the cooling curves, TEM PRO CUR and PRE PRO CUR are optional.

PROduct CURve =

Request cooling curves for products. Enter either a 0 or a 1 for each product in top-to-bottom order: 0 to print curve; 1 to suppress curve

TEMperature PROduct CURve (T units) =

Optionally, specify the lower and upper temperature limits for each product. Enter two values per product. (default lower limit is 100 F and default upper limit is product temperature)

PREssure PROduct CURve (P units) =

Optionally, specify the lower and upper pressure limits for each product. Enter two values per product. (default is product pressure for both limits)

Example: Request cooling curves for the third and fourth products.

```
PRO CUR = 1,1,0,0
```

Example: Cooling curves are to be printed for two products. Specify lower temperature limits of 25 and 100 C for the first and second products. Also, specify a pressure range of 22 and 24 PSIA for the first product and 28 to 30 PSIA for the second.

```
PRO CUR = 0,0
```

```
TEM PRO CUR (C) = 25,0,100,0
```

```
PRE PRO CUR = 22,24,28,30
```

Pumparound cooling curves

You can request cooling curves to be printed for one or more pumparounds and optionally specify the temperature and pressure ranges for each curve with these commands. Only PRO PUM CUR is required for the cooling curves, TEM PUM CUR and PRE PUM CUR are optional.

PROduct PUMparound CURve =

Request cooling curves for pumparounds. Enter either a 0 or a 1 for each pumparound in top-to-bottom order: 0 to print curve; 1 to suppress curve

TEMperature PUMparound CURve (T units) =

Optionally, specify the lower and upper temperature limits for each pumparound. Enter two values per pumparound. (default lower limit is 100 F and default upper limit is pumparound draw temperature)

PREssure PUMparound CURve (P units) =

Optionally, specify the lower and upper pressure limits for each pumparound (two values per pumparound, default is pumparound pressure for both limits)

Example: Request cooling curves for the first and third pumparounds.

```
PRO PUM CUR = 0,1,0
```

Example: Request cooling curves to be printed for two pumparounds. Specify temperature ranges of 90 to 250 F for the first pumparound product and 125 to 400 F for the second. Also, specify pressure ranges of 1.5 to 1.7 atmospheres for the first pumparound product and 2.0 to 2.75 atmospheres for the second.

```
PRO PUM CUR= 0,0
```

```
TEM PUM CUR= 90,250,125,400
```

```
PRE PUM CUR (ATM) = 1.5,1.7,2.0,2.75
```

Product IBP and EP Volume Percents

For various products, the actual IBP or EP is not a meaningful value and the 1 or 2% point or the 98 or 99% point may be preferred. In these circumstances the output report can be adjusted to report a selected point from the curve as IBP or EP.

PROduct IBP volume percent =

Enter an initial boiling point (IBP) for each product stream. These will be used on output reports of TBP and ASTM distillation curves for the products.

PROduct EP volume percent=

Enter an end point (EP) for each product stream. These will be used on output reports of TBP and ASTM distillation curves for the products.

Example: Set PROduct IBP volume percent for product streams 1 and 2 to 1% and product streams 3 and 4 End Point to 98%.

```
PRO IBP = 1,1,0,0
```

```
PRO EP = 0,0,98,98
```


The related GENERAL section commands PRO IBP and PRO EP, set one value for IBP for all product curves (TBP and ASTM) and one value for EP for all product curves.

Refine: Column Profiles

It may be helpful to enter column profiles for two purposes:

- To set non-linear pressure profiles or special solubility data profiles for unusual cases, for example - vacuum columns or quench columns. These are profiles which are **set values**.
- To improve the initial starting profiles of an unconverged column or an otherwise difficult to converge column. These are profiles which are **initial estimates** only.

Refine: Profiles Which are Initial Estimates Only

DESIGN II automatically sets up an initial column profile based on the values you enter for TEMperature of TOP, TEMperature of BOTtom, and product flowrates. In rare cases, the column may fail to converge from those initial estimates. In such cases, the column profile commands are used to enter stage-by-stage profiles for temperatures, vapor or liquid traffic and water mole fractions. These profiles are used as initial guesses only but should be used only after review of the printout from an unconverged run with a fairly clear idea of what caused the nonconvergence.

All commands are entered for each stage in top-to-bottom order, main column first then side strippers with zeroes for linear interpolation. Remember that the PROfile must be consistent with other commands used to specify or estimate stage temperatures.

TEMperature PROfile (T units) =

Enter initial temperature guesses for each stage. Do not include total condensers.

VAPor PROfile (molar Q units/t units) =

Enter initial values for vapor rates for each stage. Do not include total condensers. The vapor profile rates include steam.

LIQuid PROfile (molar Q units/t units) =

Enter initial guesses for total liquid leaving each stage. Include flow from the condenser for the TOT column type. Do not enter both vapor and liquid profiles. Vapor profiles are preferred.

P-S =

Enter estimate for mole fraction of water in the bulk liquid for each stage. Include total condensers. This command is required when modeling columns where significant "free" water will appear on any tray (except condenser), such as quench columns. This command is also required for water pumparounds and water side draws.

Temperature Profiles

DESIGN II automatically sets up temperature profiles based on values entered for TEMperature TOP and TEMperature BOTtom. If the column fails to converge with these estimates it may be beneficial to enter temperature profiles for each stage. For vacuum columns with steam, TEMperature PROfile is recommended to indicate the large temperature jump typically found between trays 1 and 2 or where similar large non-linear temperature steps are found.

Do NOT enter a value for the condenser for TOT and PUM TOT column types.

NOTE: Temperature profiles control material balance (i.e., composition on each stage) while vapor profiles control heat balance.

Example: Enter temperature profile and do not include the condenser.

TOT

STA = 21, 3, 3

TEM PRO = 120, 200, 233, 346, 466, 502, 4*0, 625, 640, 4*0, 707, 724, 739, 742, 716, 517, 506, 494, 600, 596, 588

Do not end a line with an interpolation for zeroes; for example,

wrong: TEM PRO = 200, 300, 350, 400, 4*0, 500

right: TEM PRO = 200, 300, 350, 400, 4*0, 500

Vapor Profiles

Most columns will converge starting with the initial vapor profile calculated by DESIGN II based on PROduct rate specifications or guesses. If your column does not converge, you may set up an initial vapor profile. Use the VAP PRO command to enter your guesses for total vapor leaving each equilibrium stage, in top-to-bottom order. Occasionally DESIGN II will stop, because negative liquid rates are calculated during the initialization of the profiles. VAP PRO may be used to avoid this. For the PARTIAL condenser and PUM PAR column types, the first entry must be consistent with overhead vapor product rate estimates or specifications given on the PROduct command or as implied by overall material balance for the first (top) product. A column with REFlux ratio and TEMperature of CONDenser as specifications will require either a VAPor PROfile or a PROduct rate GUEss to start the calculation. DESIGN II usually generates the vapor profile from the PROduct rate command.

Do NOT enter a value for the condenser for TOT and PUM TOT column types.

The vapor profile rates include steam.

Example: Enter vapor profile

VAP PRO (KGMOL/HR) = 4204.5, 4847, 4830, 4600, etc.

Liquid Profiles

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A liquid profile should not be used to correct negative liquid rates. They are due to a heat problem (feed too cold, too much heat removed in pumparounds).

For a TOTal condenser column type, the first entry with this command must be the estimated gross liquid flowrate from the condenser. Do not enter both a VAPor PROfile and a LIQuid PROfile. If a VAPor PROfile command is also entered, it will override the LIQuid PROfile command.

Example: Enter liquid profile

```
LIQ PRO (GMOL/SEC) =33.2, 34.0, 34.3, etc.
```

Water Mole Fraction (P-S) Profiles

A quench column (significant amount of free water present on several trays for the purpose of removing heat) requires a reasonable guess for the mole fraction of water in the bulk liquid for each stage.

A value of zero for the water mole fraction is reasonable for the stages below the last water decant.

Example: Enter water mole fraction profile for a quench column

```
P-S = .99, .988, .982, 7*0
LOC SID= 3, 3
LOC SID WAT = 3, 0
LOC PUM = 3, 1, 3, 3, 8, 7
LOC PUM WAT = 0, 0, 1
STA = 10
```

Refine: Profiles Which are Set Values

Of the values which may be set, the most common is PREssure. Pressure profiles are normally required only for low-pressure or vacuum distillation columns, for which the pressure profile is often nonlinear. The solubility profile commands are typically used when modeling a quench column.

The K-value profile command allows you to set the K-values versus stages for specific components. All commands are entered for each stage in top-to-bottom order, main column first then side strippers. Zeroes are allowed for linear interpolation. Remember that the PROfile must be consistent with other commands used to specify or estimate stage temperatures.

PREssure PROfile (P units) =

Enter values for pressures for each stage. Include a value for total condensers.

K-S = i, data

Enter K-values for component "i" for each stage, where "i" is the position in the COMponents list. Include a value for total condensers.

S-S = i, data

Enter the component solubility in the bulk liquid phase for component "i" on each stage, where "i" refers to the position in the COMponent list.

Pressure Profiles

If pressure profiles are not entered, the profile is assumed to be linear from top to bottom and is calculated from your entries for PREssure of TOP and DELta pressure. Be sure you include a pressure for any condenser, if present.

Example: Enter pressure profile

```
PRE PRO (ATM) = 1.70, 1.71, 1.73, 1.74, etc.
```

Component K-values (K-S) Profiles

You can enter K-values for a component for each stage in the REFIne module. If fewer K-values are entered than there are stages, the last value will be used for the remaining stages (including stages). An alternative method for overriding predicted K-values for one or more components is to enter K-value versus temperature (K-T) data via the ChemTran program.

Example: Enter K-values for the third (3) component

```
K-S = 3, 1.4, 1.5, 6*1.4, 10*1.5, 10*1.6, 5*1.7
```

Component Solubility (S-S) Profiles

This command is primarily for entering water solubilities in hydrocarbons, if you choose to override the calculation technique specified in the GENeral section.

Example: Enter water solubility data (water is first in COM list)

```
S-S = 1, 0.00038, 0.009, 0.0095, 0.01, etc.
```

Refine: Convergence Control

These two commands are used to control the degree of convergence of the column. Their default values are normally

adequate but may be overridden if desired.

TOLerance =

Enter the maximum acceptable NORM for the column. The NORM is the error in the tray heat and material balance on a fractional basis squared. The default is TOL=0.1E-4 or about 0.3% average error.

MAXimum MATrices =

Enter the maximum number of matrix inversions for column solution. Default is 5. Maximum recommended value is 6.

The simultaneous solution technique used in REFIne normally permits rapid convergence with the default setting. However, on some difficult or poorly specified columns, REFIne may come close but not converge on the first matrix inversion. In cases where the final iteration's NORM is .1E-2 or smaller, a MAX MAT=6 will use more computer time but often reach converge solutions.

Refine: Column REStart Capability

REFine Section Commands

The REFIne unit operation is required to solve large sets of nonlinear algebraic equations and for complex towers this can be time consuming. To improve engineering productivity, the REStart feature can be used to speed execution of multiple cases of REFIne columns. The solution of the nonlinear algebraic equations for a REFIne column is stored in a file and subsequent runs of the REFIne column can read this file and restart the calculations from the column's previous solution. The restart option may be used for a column which has the same physical configuration and specifications as the original column although the values of the specifications may be different.

Using the REStart feature can reduce the runtime by more than 50%. Enter one of the following optional commands in the REFIne module.

WRite to REStart FILE

Writes restart information to the file named in the GENeral section.

LOAd from REStart FILE

Reads restart information from the file named in the GENeral section.

Refine: GENeral Section Commands

Enter one of the following commands in the GENeral section.

NEW REStart FILE = name

Enter any name of the restart file when using the WRite REStart FILE command in the REFI unit. This creates the file where the solution to the REFIne column is written.

OLD REStart FILE = name

Enter any name of the restart file when using the LOAd REStart FILE command in the REFI unit. This opens an existing file from which restart data can be read or written.

Refine: Application of Commands

The WRite REStart FILE and LOAd REStart FILE commands operate in conjunction with the NEW REStart FILE or the OLD REStart FILE command according to the following rules:

1. Load (read) operations initiated by the LOA REStart FILE command will always be done on the file named in the OLD REStart FILE command.
2. If only the OLD REStart FILE command is present in the GENeral section, then the write operation is performed on the file named in this command and the old data is overwritten.
3. If both the OLD REStart FILE and the NEW REStart FILE command are present, then the write operation is performed on the file named in the NEW REStart FILE command.

Refine: Restrictions

There are certain restrictions on how the restart option may be used:

1. Restart information from a previous column calculation should be used only for a column that has the same physical configuration and specifications. The actual values of the specifications may be changed. For example, the locations of side strippers, side draws, the number of trays in either the main column or in side strippers **must** remain the same. The less the specification values are changed, the faster the execution time.
2. No parameter should be changed that alters the problem description. Although product rate specifications may change, all specification types must remain the same. For example, the value of a column FIX may be changed, however, the FIX specification itself may not be added or deleted. The column type must also remain the same.

Refine Distillation Columns Command Summary

Column Type

TOTAL condenser
 PARTIAL condenser
 PUMparound with TOTAL condenser
 PUMparound REFlux
 PUMparound with PARTIAL condenser

Required Column Description

STAgEs =
 TEMperature of TOP (T units) =
 TEMperature of BOTtom (T units) =
 PREssure of TOP (P units) =
 DELta pressure (P units) =
 LOCation of FEEds =

Specification Commands

PROduct rate (Q units/t units) =
 PROduct rate GUEss (molar Q/t units) =
 DUTy of condenser (H units/t units) =
 REFlux ratio =
 TEMperature of CONDenser (T units) =
 PROduct OVERhead rate (Q units/t units)=
 HEAt from PUMparound (H units/t units)=
 FIX TEMperature of top tray (T units)=

Side Draws

LOCation of SIDedraws =
 LOCation of SIDedraws for WATER =

Condenser

PREssure of CONDenser (P units) =
 TEMperature of CONDenser (T units) =
 TEMperature of CONDenser SUBcooling
 TEMperature of CONDenser GUEss (T units)

Side Strippers

LOCation of DRAws =
 LOCation of VAPor returns =
 LOCation of LIQuid returns =
 PROduct from STRipper (Q units/t units)=
 DRAwrate to strippers (molar Q units/t units) =
 RETurn flow from stripper (molar Q units/t units) =
 PROduct from STRipper GUEss (molar Q/t units) =
 HEAt from RETurn (H units/t units) =
 TEMperature of RETurn (T units) -
 CHAnge in RETurn temperature (T units) =

Steam

LOCation of STEam =
 PREssure of STEam (P units) =
 TEMperature of STEam (T units) =
 STEam rates (Q units/t units) =

Reboilers

REBoiler TYPE =
 REBoiler duty (H units/t units)=
 REBoiler EXIt VAPorization percent=
 REBoiler FLOWrate (Q units/t units) =
 REBoiler duty (H units/t units)=
 REBoiler VAPor GUEss (molar Q units/t units) =
 REBoiler return DELta pressure (P units) =
 REBoiler NAME =

Heater and Coolers

LOCation of HEATers =
 HEAt added or removed (H units/t units) =

Refine Restart Capability

Pumparounds

LOCation of PUMparounds =
 LOCation of PUMparound for WATER =
 PROduct of PUMparound (Q units/t units) =
 HEAt from PUMparounds (H units/t units) =
 TEMperature of PUMparounds (T units) =
 CHAnge of PUMparound temperature (T units) =
 PROduct PUMparound GUEss (molar Q/t units) =

FIX Tray Conditions

FIX GUEss (molar Q units/t units) =

Internal Stream Commands

INT CON STR = x, -y
 INT CON SEP = x, -y
 INT CON DEC = x,
 INT REB STR = x, -y,
 INT HEA STR INO = x, -y
 INT FEE HEA INO = x,
 INT PUM STR INO = x, -y
 INT STR STR INO = x, -y (OR)
 INT STR STR INO = x, -y, -z
 INT STR REB INO = x, -y

Tray Sizing

SPACing of TRAYs (L units) =
 WEIr HEIght (L units) =
 WEIr LENGth (L units) =
 DOWNcomer AREa (L2 units) =
 GLItsch SYStem factor =
 GLItsch PERcent flood =
 GLItsch SWAge trays =
 GLItsch PASses per tray per section =
 GLItsch SPACing per tray per section (L units) =
 GLItsch DIAMeter per tray per section (L units) =
 GLItsch DOWNcomer AREa per tray per section (L2 units) =
 GLItsch WEIr HEIght per tray per section (L units) =
 GLItsch VALve TYPE =
 GLItsch VALve MATERIAL =
 GLItsch VALve THICKness (L units) =
 GLItsch VALve NUMber (1/L2 units) =
 GLItsch DECK thickness (L units) =

Calculation Options

FENSke calculation
 HKEy=
 KKEy=
 DKEy=
 IMMiscible=
 NO IMMiscible

Print Options

SMITH SIZing OFF
 GLItsch SIZing OFF
 COLumn SIZing OFF
 REPorts =
 CONDensing CURve
 PLOT OFF
 SWItch =
 PROduct NAMES =
 PROduct CURve =
 TEMperature PROduct CURve (T units) =
 PREssure PROduct CURve (P units) =
 PROduct PUMparound CURve =
 TEMperature PUMparound CURve (T units) =

WRITE to REStart FILE
LOAD from REStart FILE
 (used in conjunction with NEW RES FIL = & OLD
 RES FIL = commands...See Refine: GENeral
 Section Commands)

Convergence Control

TOLerance =
MAXimum MATrices =

PREssure PUMparound CURve (P units) =
PROduct IBP volume percent =
PROduct EP volume percent =

Profiles Which Are Initial Estimates Only

TEMperature PROfile (T units) =
VAPor PROfile (molar Q units/t units) =
LIQUid PROfile (molar Q units/t units) =
P-S =

Profiles Which Are Set Values

PREssure PROfile (P units) =
K-S = i, data
S-S = i, data

Refine Distillation Columns Step by Step

Refine Distillation STEP 1

Enter all the information at the right to uniquely define the module and its connections to the rest of the flowsheet.
 Equipment name and connectivity (ALL are required).

equipment module identifier
 equipment number
 equipment name
 inlet stream(s)
 outlet streams

REFI

assigned equipment flowsheet number
 user choice - up to 16 characters
 unlimited number, in top-to-bottom order
 unlimited number, in top-to-bottom order

Stream number conventions

- water decanted from condenser is not numbered
- steam feed are not numbered
- pumparound draws and returns are not numbered

Refine Distillation STEP 2

Select one column type from the five main configurations. See Refine Distillation Column Type.

Main column types (select ONE)

reflux from total condenser, no vapor to product	TOT
reflux from partial condenser, vapor top product, optional liquid top product	PAR
reflux from pumparound, vapor top product	PUM REF
reflux from pumparound, no vapor top product	PUM TOT
reflux from pumparound, vapor and liquid top products	PUM PAR

Refine Distillation STEP 3

Enter the required column description.

Required column description (enter ALL of the following).

NOTE: A partial condenser is stage 0. The top tray is always numbered 1.

number of equilibrium **stages** for main column then each side stripper, separated by commas in top-to-bottom order. (example: STA25,3,3) "**Stages**" includes partial condensers, theoretical trays and reboilers. A total condenser is not a stage.

top tray temperature guess (multiple values allowed)

bottom product temperature guess (multiple values allowed)

top tray pressure (multiple values allowed; side strippers in top to bottom order)

column pressure drop (default is 0; multiple values allowed; side strippers in top to bottom order)

feed **tray** locations (enter tray numbers separated by commas in top-to-bottom order). Number the **trays** (including any reboilers) in top-to-bottom order starting with the main column then each side stripper. Tray 1 is the top tray of the main column. Stage 0 is the condenser, if present. Liquid portion of feed mixes on the feed tray and vapor portion of feed mixes on the tray above the feed tray

STA =

TEM TOP (T units) =

TEM BOT (T units) =

PRE TOP (P units) =

DEL (P units) =

LOC FEE =

Refine Distillation STEP 4

Select heat and material balance specification(s).

Choose the number of specifications required based on the column type.

Column type	Minimum Number of Specifications Required
TOT	1 specification
PAR	2 specifications
PUM REF	1 specification
PUM TOT	1 specification
PUM PAR	2 specifications

Quick Reference Table of Allowable Specifications

Column Type	Number Required	PRO	DUT	REF	TEM CON	PRO OVE	HEA PUM	FIX TEM
TOT	1	X	X	X				
PAR	2	X	X	X	X	X		
PUM REF	1	X		X			X	X
PUM TOT	1	X		X			X	X
PUM PAR	2	X	X	X	X	X	X	X

Select specification(s) from the following options

(Refer to the table on the preceding page for allowable specifications based on column type. If more than the required number of specifications is given, then, the specifications used are **Refine: Hierarchy of Heat and Material Balance Specifications.**)

Product flowrates in molar, mass, or volume units. Enter values separated by commas for unstripped products from the main column in top-to-bottom order. Use zeros for unspecified flowrates to maintain order. Products include vapor distillate (PAR, PUM PAR and PUM REF), liquid distillate (TOT, PAR, PUM TOT and PUM PAR), unstripped side draws (including "free water draws excluding condenser water") and bottom product. At least one of the distillate or bottoms flowrates must be zero. Flowrates for unstripped side draws are always required. Non-zero values of vapor distillate, liquid distillate and bottoms distillate are used as specifications

reflux ratio

condenser duty

temperature of condenser outlet

total distillate (vapor and liquid) overhead product flowrate only allowed if TEM CON also specified)

heat removed by the top pumparound (PUM REF, PUM TOT, PUM PAR only). (See pumparound commands in **Refine Distillation STEP 10**)

fix the top tray temperature by varying the duty of the pumparound returning to the top tray (PUM REF, PUM TOT, PUM PAR only). See FIX commands in STEP 11.

PRO (Q units/t units) =

REF =

DUT (H units/t units) =

TEM CON (T units) =

PRO OVE (Q units/t units) =

HEA PUM (H units/t units) =

FIX TEM (T units) i =

Optional molar product flowrates

if product flowrates are entered in mass or volume units, then molar flowrates should be entered for as guesses all unstripped products

PRO GUE (molar Q units/t units) =

Refine Distillation STEP 5

Specify optional column description.

Side draw locations.

Tray locations of unstripped side draws including water decants from trays. Do not include water decant from condenser. Enter in top-to-bottom order, separated by commas. Negative numbers indicate vapor draws

LOC SID =

Tray locations where free water is to be decanted from trays (not including decant from condenser). Enter zeros for any side draw locations which are for hydrocarbon products to maintain top-to-bottom order

LOC SID WAT =

Condenser Options

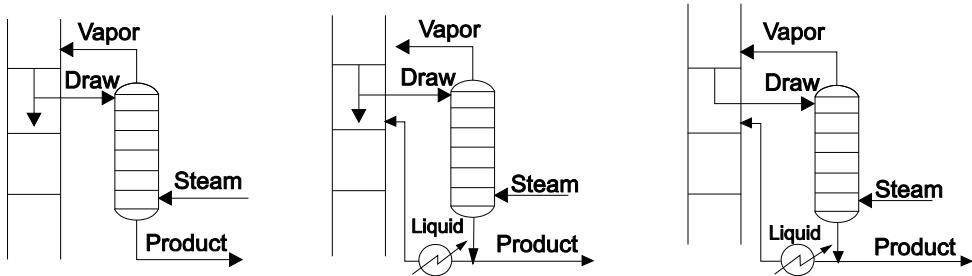
- Pressure out of condenser (default is top tray pressure)
- Condenser temperature (for TOT and PUM TOT column types only)
- Degrees of condenser subcooling (for TOT and PUM TOT column types only)
- Condenser temperature guess (for TOT and PUM TOT column types only)

- PRE CON (P units) =
- TEM CON (T units) =
- TEM CON SUB (T units) =
- TEM CON GUE (T units) =

Refine Distillation STEP 6

Describe side strippers if present.

Types of side strippers



A. Partial draw with no liquid return B. Partial draw with liquid return C. Total draw with liquid return

Required side stripper description

(Enter ALL of the following to describe each stripper; enter tray locations in top-to-bottom order, separated by commas.)

- Tray locations in main column for liquid draws to each stripper LOC DRA =
- Tray locations in main column for vapor returns from each stripper (vapor mixes in tray above return location) LOC VAP =
- Tray locations in main column of liquid returned from each stripper (only enter if liquid is returning to main column) LOC LIQ =

Required side stripper specifications

(Enter one or two specifications for all strippers according to the quick reference table below. Enter zeroes to maintain top-to-bottom order.)

Quick reference table of stripper specifications

Stripper Type	Number Required	Allowable Specifications "X"		
		PRO STR	DRA	RET
A. partial draw, no return	1	X	X	
B. partial draw, with liquid return	2	X	X	X
C. total draw, with liquid return	2	X	X	X

- Product flowrates from strippers in molar, mass or volume units PRO STR (Q units/t units) =
- Draw rates from main column in molar units or the fraction of liquid drawn from tray, fraction of 1 implies total draw DRA (molar Q units/t units or FRA) =
- Return liquid molar flowrates from strippers to main column in molar units RET (molar Q units/t units) =

RECOMMENDED: If PRO STR in mass or volume units, then enter molar guesses

- Stripper product flowrate guesses in molar units PRO STR GUE (molar Q units/t units) =

OPTIONAL: If stripper has a liquid return, then return liquid cooling may be specified (enter one specification per liquid return, enter zeroes to maintain top-to-bottom order)

- Heat removed from return liquid stream HEA RET (H units/t units) =
- Temperature of returned liquid stream TEM RET (T units) =
- Temperature drop of returned liquid stream CHA RET (T units) =

Refine Distillation STEP 7

Specify main column and side stripper heat sources.

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Main column and each side stripper must have a bottom heat source.

- Steam (STEP 7)
- Reboiler (see *Refine Distillation STEP 8*)
- Vapor feed stream below bottom tray (see *Refine Distillation STEP 3*)
- Tray heater (see *Refine Distillation STEP 9*)

Steam heat sources (enter ALL of the following)

(enter values for all steam feeds in top-to-bottom order)

Steam feed tray numbers (tray number just below tray where steam enters)

Steam feed pressures

Steam feed temperatures

Steam feed flowrates

LOC STE =

PRE STE (P units) =

TEM STE (T units) =

STE (Q units/t units) =

Refine Distillation STEP 8

Specify reboiler heat sources if present.

See *Refine: Reboilers*. to Identify **type** for each reboiler.

(Enter value for main column first, then values for each side stripper in to-to-bottom order, separated by commas. Use zeroes to maintain order if a column has no reboiler.)

Kettle (default)

REB TYP = 1

Thermosiphon (recirculating)

REB TYP = 2

Hot draw recirculating

REB TYP = 3

Enhanced recirculating

REB TYP = 5

If type 1 reboiler, enter required specification (Enter duties for main column first, then each side stripper, use zeroes to maintain order.)

Reboiler duties

REB (H units/t units) =

If type 2, 3 or 5 reboiler (select two specifications) (Enter for main column first, then each side stripper, use zeroes to maintain order. If more than 2 specifications entered for any reboiler, the first two in the list below will be specifications the others will be initial guesses. Negative values can be used to indicate initial guesses.)

Reboiler exit weight percent vaporized

REB EXI VAP =

Reboiler inlet liquid flowrates

REB FLO (Q units/t units) =

Reboiler duties

REB (H units/t units) =

Reboiler outlet temperatures

REB TEM (T units) =

• Required initial guesses (for each such reboiler, enter a negative value to indicate an initial guess if a positive value has not already been specified above)

Reboiler liquid flowrates

REB FLO (Q units/t units) =

Reboiler duties

REB (H units/t units) =

• Optional commands

Reboiler return line pressure drop

REB DEL (P units) =

Initial guess of reboiler vapor returning to the column

REB VAP GUE (molar Q units/t units) =

Reboiler names, up to 16 characters each

REB NAM

Refine Distillation STEP 9

Specify tray heaters and coolers.

Tray heaters and coolers (if present, enter BOTH commands)

(enter values separated by commas in top-to-bottom order)

Tray numbers on which the tray heaters and coolers are located

LOC HEA =

Duties for heaters and coolers (positive for heating, negative for cooling)

HEA (H units/t units) =

Refine Distillation STEP 10

Specify pumparounds, pumpups and pumpdowns.

Location of pumparounds.

Enter draw tray and return tray for each pumparound separated by commas, top pumparound values first followed by second pumparound and so on. Negative return values “-n” indicate return to the “nth” feed to the column (counting from the top)

LOC PUM =

If there are free water pumparound(s), then enter one value for each pumparound: either 1 for pure water or 0 for hydrocarbon in top-to-bottom order

LOC PUM WAT =

Pumparound specifications (enter TWO of the following for each pumparound)

(Each command will have entries for all pumparounds. Enter a zero for each pumparound to which a specification does not apply. This will maintain top-to-bottom order.)

Pumparound flowrates. Negative values indicate estimates only, not specification and

PRO PUM (Q units/t units) =

Pumparound molar flowrate guesses if PRO PUM is in mass or volume units (recommended)

PRO PUM GUE (molar Q units/t units) =

Pumparound duties

HEA PUM (H units/t units) =

Pumparound return temperatures

TEM PUM (T units) =

Pumparound temperature drops

CHA PUM (T units) =

Refine Distillation STEP 11

Specify optional FIXES on tray conditions.

FIX a tray parameter by varying a tray duty, heater duty or product flowrate.

(enter one command for each “fixed “ parameter)

Command syntax

FIX parameter (units) **i** = value, tray, variable

parameter can be:

LIQuid rate (total) from a tray

LIQuid rate **NET** from a tray (after satisfying draw rate and pumparound)

VAPor rate (total) from a tray

TEMperature of a tray

Units

refers to dimensional units of the specified value

i

is a number from 1 to n, each fix is numbered in top to bottom order.

Value

is the desired value of the fixed parameter

Tray

is the tray number being fixed of 0 for condense

variable can be:

a duty on a tray, enter tray number

a feed heater, enter **H** and a feed number

product flowrate, enter **P** and a product number in top to bottom order based on draw location

RECOMMENDED: Molar flowrate guesses

If one or more FIX commands for flow rates are given in mass or volume units, then molar guesses must be in top-to-bottom order, separated by commas

FIX GUE (molar Q units/t units) =

Refine Distillation STEP 12

Specify optional product specifications.

Meet a product property specification by varying a product rate.

(enter one command for each product specification)

Command syntax

PRO SPE (units) **j** = value, property, product, variable

units

refers to dimensional units of the specified value

j

is a number from 1 to n, PRO SPEs are numbered in top to bottom order based on product draw location.

value

is the desired value of the property specified

property

can be properties such as **ASTM IBP** listed in *Property Keyword Table* below

product

can be:

PRODn

where “n” is the product number (in top-to-bottom order) of the product to which the specification applies

variable

can be:

PRODn

where “n” is the product number (in top-to-bottom order) of the product whose rate will be varied to meet the specification

Product Property Keyword Table

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ASTM IBP	D-86 initial boiling point (2%)
ASTM 5PT	D-86 5% point
ASTM 95PT	D-86 95% point
ASTM EP	D-86 end point (98%)
ASTM GAP	D-86 5% point of the next heavier product minus the 95% point of the specified product
TBP IBP	TBP initial boiling point (2%)
TBP 5PT	TBP 5% point
TBP 95PT	TBP 95% point
TBP EP	TBP end point (98%)
PUR COM n	mole fraction in specified product of the nth component in the COMponent list
PUR COM n TO m	total mole fraction in specified product of the nth to mth components in the COMponents list.
AMW	average molecular weight
GRA	average gravity
FLA	flash point
FLO	mass or volume flow rate (you must specify mass or volume units for this option)
VIS SET n	viscosity from the nth user provided viscosity data set
PRO SET n	user entered property from the nth user entered property data set
POUR	pour point from the user entered pour point data

Refine Distillation STEP 13

Select a shortcut tray sizing options.

Smith-Dresser-Ohlswager technique (All optional) (enter all commands to replace 18 inch default setting height)

Spacing of trays	SPA TRA (L units) =
Weir height	WEI HEI (L units) =
Weir length	WEI LEN (l units) =
Downcomer area (default is 12% of empty column area)	DOW ARE (L2 units) =

Glitsch technique (all optional) (Enter GLI PER to calculate diameters or enter GLI DIA to calculate percent flood. Do not enter both GLI PER and GLI DIA)

System factor for foaming (one value, default is 1)	GLI SYS =
Percent of flood (one value, default is 80%)	GLI PER =
Number of tray passes (one value: 1,2, or 4 passes). In REFine columns only, GLitsch PASSes can be different and should correspond to the number of GLitsch SWAge trays plus one.	GLI PAS per tray per section =
Tray spacing(s) (default is 2 feet)	GLI SPA per tray per section (L units) =
Diameter(s) of trays	GLI DIA per tray per section (L units) =
Tray number(s) immediately below swage (for columns with more than one diameter or spacing)	GLI SWA =
Enter the total downcomer area per tray. Will be calculated, when not provided.	GLI DOW ARE per tray per section (L2 units) =
Enter the weir height to be used along with GLitsch SPACING in calculating the settling height. Default is 3 inch	GLI WEI HEI per tray per section (L units)=
Enter the valve type. Either 1 or 4 is available. Default is 1.	GLI VAL TYPE =
Enter the valve material. Default is carbon steel.	GLI VAL MAT =
Enter the valve thickness. Default is 0.06 inch.	GLI VAL THI (L units) =
Enter the number of valves per square foot. Default is 13.	GLI VAL NUMBER 1/L2 units) =
Enter the deck thickness. Default is 0.104 inch.	GLI DECK thickness (L units) =

Tray sizing print options

Delete Smith-Dresser-Ohlswager calculation and output	SMI SIZ OFF
Delete glitsch calculation and output	GLI SIZ OFF
No column sizing output	COL SIZ OFF
Tray number(s) immediately below swage (for columns with more than one diameter or spacing)	GLI SWA =

Refine Distillation STEP 14

Select calculation and print options.

Fenske shortcut material balance

Perform a Fenske shortcut material balance calculation only; NOT the rigorous tray-by-tray calculation	FEN
If thermo is different than global (GENeral section), THEN select	
K-value option	KKE =
Enthalpy option	HKE =
Density option	DKE =
Control Column Output	
Suppress selected sections of output report. Enter six values separated by commas (default is REP=0,0,0,0,0,0). Enter a 0 to print or a 1 to suppress print of sections as follows	REP =
first entry = 1 deletes tray-by-tray compositions and K-values	
second entry = 1 deletes feed flash summary	
thirdentry = 1 deletes product volume percents, mole, mass and volume rates	
fourth entry = 1 deletes product gravities, molar, mass and volume rates	
fifth entry = 1 deletes property, temperature, vapor and liquid profiles	
sixth entry = 1 deletes API viscosity profiles	
Print control	
Request condensing curve	CON CUR
Suppress plots of TBP & ASTM curves for products	PLO OFF
Column convergence information, enter 0 to suppress print or 1 to print or 2 for diagnostic printout (default is 1)	SWI =
Identify product names. Enter product names separated by commas based on draw location in top-to-bottom order. Maximum of 16 characters per name. NO continuation lines are allowed	PRO NAM =
Product cooling curves	
Request cooling curves for products. Enter either a 0 or a 1 for each product in top-to-bottom order: 0 to print curve; 1 to suppress curve	PRO CUR =
Optionally, specify the lower and upper temperature limits for each product. Enter two values per product. (default lower limit is 100 F and default upper limit is product temperature)	TEM PRO CUR (T units) =
Optionally, specify the lower and upper pressure limits for each product. Enter two values per product.(default is product pressure for both limits)	PRE PRO CUR (P units) =
Pumparound cooling curves	
Request cooling curves for pumparounds. Enter either a 0 or a 1 for each pumparound in top-to-bottom order: 0 to print curve; 1 to suppress curve	PRO PUM CUR =
Optionally, specify the lower and upper temperature limits for each pumparound. Enter two values per pumparound. (default lower limit is 100 F and default upper limit is pumparound draw temperature)	TEM PUM CUR (T units) =
Optionally, specify the lower and upper pressure limits for each pumparound. Enter two values per pumparound. (default is pumparound pressure for both limits)	PRE PUM CUR (P units) =

Refine Distillation STEP 15

Enter optional column profiles and convergence control parameters.

Profiles which are initial guesses (normally not needed).

(use notations for repetition, (5*300), interpolation, (10*0) and exponents, (3.5E5), if desired)

Temperatures for each stage (do NOT include total condenser)	TEM PRO (T units) =
Vapor flowrates for each stage (do NOT include total condenser)	VAP PRO (molar Q units/t units) =
or	
Liquid flow for each stage (include total condenser)	LIQ PRO (molar Q units/t units) =
Mole fraction water in bulk liquid for each stage for columns with water decants in addition to automatic condenser decant (includes total condenser)	P-S =

Profiles which are set values

(use notations for repetition, (5*300), interpolation, (10*0), and exponents, (3.5E5), if desired)

Pressure of each stage (include total condenser)	PRE PRO (p units) =
--	----------------------------

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K-values for component "i" for each stage (include total condenser) where "i" is the position in the Component list

K-S = i, data

Component solubility in bulk liquid phase for component "i" for each stage (include total condenser) where "i" is the position in the Component list

S-S = i, data

Convergence control parameters

Maximum acceptable error in the heat and material balance on a fractional basis squared (default is 0.1 E-4)

TOT =

Maximum number of matrix inversions (default is 1, maximum is 6)

MAX MAT =

Refine Distillation Columns Examples

There are several sample flowsheets in "Chapter 40: Refine Column Samples - c:\designii\samples\equipmnt\refine" of the DESIGN II for Windows Tutorial and Samples Guide.

Refine Distillation Columns References

General

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7. J. R. Fair, "Comparing Trays and Packings", *Chemical Engineering Progress*, Vol. 66, Number 3, pp. 45-49 (March, 1970).
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Flash Points

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Fenske Fractionation Indices

1. R. Jakob, "Estimate Number of Crude Trays", *Hydrocarbon Processing*, Vol. 50, pp.149-152, Gulf Publishing Co., Houston, May, 1971.

Practical Use of REFINE

1. P. Baron, "Crude Oil Distillation - Practical Benefits through Process Simulation", I. Chem E. Symposium Series No 61. pp 27-40. Institution of Chemical Engineers, Rugby, England.

Chapter 37: Shortcut Fractionator

Shortcut Fractionator Features

The SHORtcut fractionator module simulates a simple distillation column with one feed and a top and bottom product. For a specified recovery of light and heavy key components, the following is estimated:

feed tray location reflux ratio number of theoretical stages condenser duty reboiler duty

This information is reported for six standard percentages of minimum reflux (105,110,120,140,170, 200%) and for another percent of minimum reflux you can specify.

An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure. Two output streams (a top and bottom product) **must** be coded.

The column is assumed to have both a condenser generating reflux, and a reboiler generating vapor. Only a top product (liquid or vapor) and a bottoms liquid product are calculated. To simulate a column with a vapor and a liquid overhead product run the column as a PARTial condenser and as a TOTal condenser and interpolate between the two results.

For other columns not having both a condenser and reboiler, you can use the COMponent SPLitter. To simulate columns with multiple products, break the column into sections each having two products, and simulate the sections individually.

The SHORtcut fractionator results are most reliable for "ideal" separations. The accuracy and reliability of the results will decrease as the degree of non-ideality increases.

Method of Calculation

The SHORtcut fractionator uses standard text book techniques in calculating feed tray location, reflux ratio, theoretical stages, and condenser and reboiler duties. The relative volatilities of the components are assumed to be constant throughout the column. The vapor and liquid rates above the feed tray are assumed constant, as are the vapor and liquid rates below the feed tray.

The following equations are used:

Shiras - for calculation of *component distribution* between the top and bottom product for components other than the light and heavy key.

Underwood - for *minimum reflux* ratio.

Fenske - for *minimum theoretical* stages.

Erbar-Maddox - for *theoretical stages* if the feed is between bubble point and dew point conditions.

Gilliland - for *theoretical stages* if the feed is subcooled or superheated.

Kirkbride - *feed tray location* (from top of column).

See sample printout in Example 1 which includes a plot of reflux versus stages required for separation.

Shortcut Fractionator Command Details

Shortcut Fractionator: Condenser Specification Commands

(enter only one)

PARTial condenser Specifies vapor top product.

TOTal condenser Specifies liquid top product.

Shortcut Fractionator: Recovery Specifications Commands

Neither 100% nor 0% recoveries can be specified (.99999 and .00001 are the mole fraction limitations). The light and heavy key components do not have to be next to each other in the order of components, nor does the light key have to be first in order. The light and heavy key component separation specified must be realistic. At least 50 percent of the light/heavy key component must go to overhead/bottoms. If the concentration of the heavy key component in the overhead product is too large, the shortcut calculation might fail, as indicated by the warning message "VAPOR FROM TOP LESS THAN OVERHEAD-- REFLUX SET EQUAL TO 1.2*OVERHEAD". The same is true for the light key in the bottom. (both must be specified)

RECovery to **TOP** **i** = fraction

Enter the fractional amount of light key component "i" in the feed that is to go to the top product.

RECovery to **BOT**tom **i** = fraction

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Enter the fractional amount of heavy key component "i" in the feed that is to go to the bottoms product.

NOTE: "i" is the component ID number of the light or heavy key.

Shortcut Fractionator Optional Command Details

Shortcut Fractionator: Operating Parameters Commands

DELta pressure (P units) =

Enter the column pressure drop. Default is zero.

PERcent of **MIN**imum reflux = *percent*

Enter the percent of minimum reflux. Default is 130.

PREssure of **TOP** product (P units) =

Enter the pressure for the top product. Default is: (feed pressure - 0.5 x DEL.)

Shortcut Fractionator: LOSt Work Commands

For LOSt work analysis, DESIGN II will use default temperatures for heat exchange calculations unless you enter the following commands:

TEMperature of **HEA**ting fluid (T units) =

Enter value for utility side of reboiler. Default is 250 F.

TEMperature of **COO**ling fluid (T units) =

Enter value for utility side of condenser. Default is 70.3 F.

Shortcut Fractionator Command Summary

Condenser Specification Commands

PARTial condenser

TOTal condenser

Recovery Specifications Commands

RECovery to **TOP** i = *fraction*

RECovery to **BOT**tom i = *fraction*

Tower Operating Parameters Commands

DELta pressure (P units) =

PERcent of **MIN**imum reflux = *percent*

PREssure of **TOP** product (P units) =

LOSt Work Commands

TEMperature of **HEA**ting fluid (T units) =

TEMperature of **COO**ling fluid (T units) =

Thermodynamics Commands

HKEy=

KKEy=

DKEy=

Shortcut Fractionator Step by Step

Shortcut Fractionator STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

SHO

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

Two only; 1st is top product, 2nd is bottom product

Shortcut Fractionator STEP 2

Choose a condenser type (enter ONE of the following options)

Partial (top vapor product)

Total (top liquid product)

PAR

TOT

Shortcut Fractionator STEP 3

Choose the top and bottom product recovery specifications (enter BOTH of the following commands)

Fractional amount of light key component in the feed with ID number "i" that is to go to the top product **REC TOP i** = *fraction*

Fractional amount of heavy key component in the feed with ID number "i" that is to go to the bottoms product **REC BOT i** = *fraction*

OPTIONAL - Column operating parameter specifications (select ANY of the following options)

Column pressure drop (default is zero)
Percent of minimum reflux (default is 130)
Pressure for the top product (default is: feed pressure - 0.5 x DEL)

IF LOST work command THEN select any of the following commands

Temperature for utility side of reboiler (default is 250 F)
Temperature for utility side of condenser (default is 70.3 F)

IF thermo is different from global (GENeral section) options THEN select

K-value option
Enthalpy option
Density option

DEL (P units) =
PER MIN = percent
PRE TOP (P units) =

TEM HEA (T units) =
TEM COO (T units) =

KKE =
HKE =
DKE =

Shortcut Fractionator Examples

There are several sample flowsheets in "Chapter 41: Shortcut Fractionator Column Samples - c:\designii\samples\equipmnt\shortcut" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 38: Spreadsheet

The SPREAdsheet module can be used to calculate an outlet stream property on a molar basis. The module can be used to modify stream component flowrates by an Excel VBA Macro. The component flowrates can be flashed to multiple outlet streams. There can be more than one inlet and one outlet streams. The spreadsheet module is solved using a Visual Basic Excel Macro (VBA) for all outlet stream conditions.

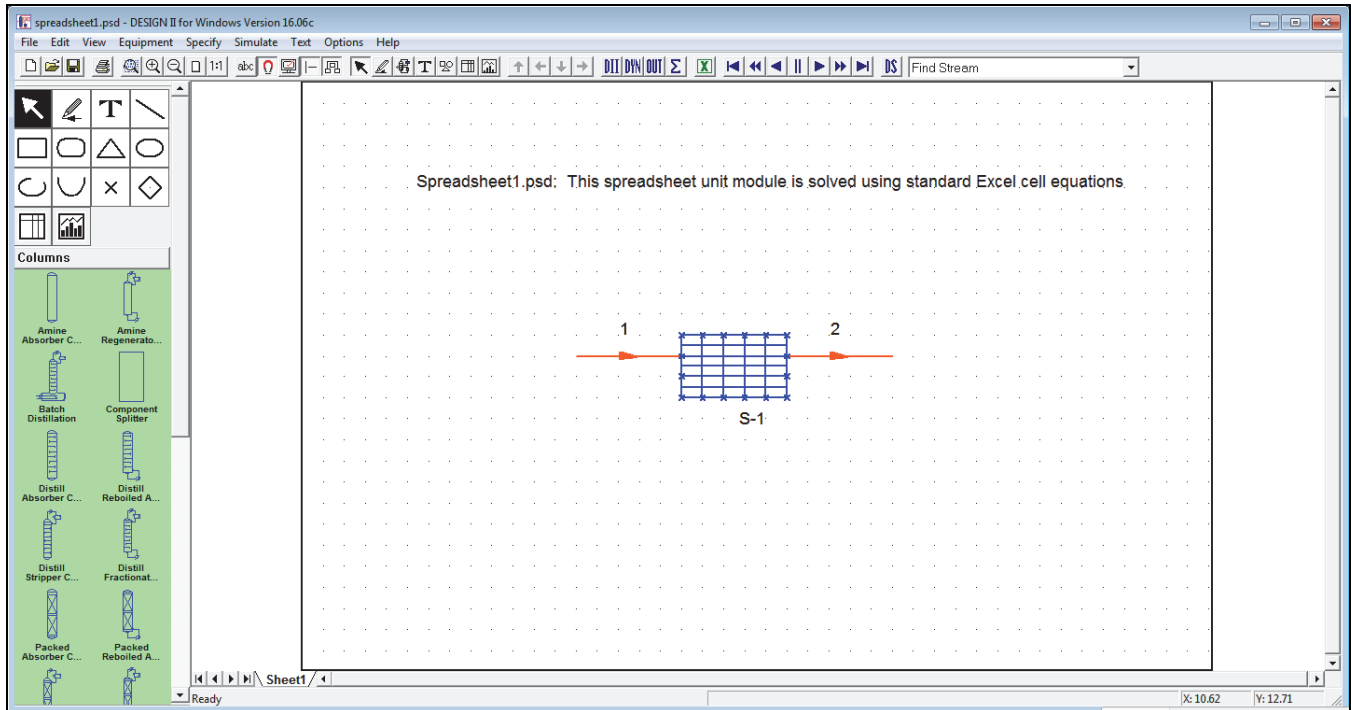


Fig. 1 Spreadsheet Spreadsheet1.psd

Spreadsheet Command Details

Spreadsheet Commands

OUT TYP SPE = 0 or 1

FIL NAM =

File Name and file path

ex: 'C:\designii\samples\equipment\spreadsheet\spreadsheet3.xlsm'

INL SHE =

Inlet Streams

INL ROW = 1

Inlet Stream Row to start

INL COL = A

Inlet Stream Column to start

OUT SHE =

Outlet Streams

OUT ROW = 1

Outlet Stream Row to start

OUT COL = A

Outlet Stream Column to start

REL SPR = 1

CAL TYP = 1

Calculation Type

MAC NAM = 'testmacro'

Macro Name

Spreadsheet Optional Command Details

UNI TEM = F
UNI PRE = psig
UNI ENTH = Btu
UNI QUA = lb
UNI TIM = hr

Spreadsheet Command Summary

Command Details

OUT TYP SPE = 0 or 1
FIL NAM =
INL SHE =
INL ROW = 1
INL COL = A
OUT SHE =
OUT ROW = 1
OUT COL = A

REL SPR = 1
CAL TYP = 1
MAC NAM = 'testmacro'

Optional Commands

UNI TEM = F
UNI PRE = psig
UNI ENTH = Btu
UNI QUA = lb
UNI TIM = hr

Thermodynamics

HKEy=
KKEy=
DKEy=

Spreadsheet Step by Step

Spreadsheet STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
Equipment number
Equipment name
Inlet stream
Outlet streams

SPRE

Assigned equipment flowsheet number
User choice - up to 16 characters
Unlimited in number
One or two; 1st copy of inlet; if two, 2nd is modified

Spreadsheet STEP 2

Choose a way to modify stream components (enter ALL of the following)

File Name and File Path
Inlet Stream
Inlet Stream Row
Inlet Stream Column
Outlet Stream
Outlet Stream Row
Outlet Stream Column

Calculation Type
Macro Name

OUT TYP SPE
FIL NAM =
INL SHE =
INL ROW = 1
INL COL = A
OUT SHE =
OUT ROW = 1
OUT COL = A
REL SPR = 1
CAL TYP = 1
MAC NAM =

Spreadsheet STEP 3

Choose Unit System

UNI TEM = F
UNI PRE = psig
UNI ENTH = Btu
UNI QUA = lb
UNI TIM = hr

IF thermo is different from global (GENeral section) options THEN select

K-value option
Enthalpy option
Density option

KKE =
HKE =
DKE =

Spreadsheet Examples

There are several sample flowsheets in “Chapter 38: Spreadsheet Samples - c:\designii\samples\equipmnt\spreadsheet” of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 39: Stream Manipulator

The STream manipulator module can be used to calculate a stream property (such as heating value) on a molar or standard vapor basis (e.g. BTU/SCF). The module can also be used to modify stream component flowrates by a single factor for all components or by an individual factor for each component. The component flowrates can be added, subtracted, multiplied, or divided by the factors. The first stream is a copy of the input. When two outlet streams are specified, the second outlet stream is the modified stream.

Stream Manipulator Command Details

Stream Manipulator Modification Operators

ADD

Add factor to component flowrates.

SUBtract

Subtract factor from component flowrate.

MULTiply

Multiply component flowrates by factor.

DIVide

Divide component flowrates by factor.

HEATING VALue

Enter this command to get the gross heating value calculated for a hydrocarbon product stream. No other calculation option is allowed.

NOTE: 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.

Stream Manipulator Modification Factor

FACTOR =

Enter factor(s) for each component flowrate. Factors must be in the same order as component ID numbers in the COMPONENT command in the GENERAL section.

Lower limit: 1E-10 - any greater value such as 1.01E-10 will work.

Upper limit: None

or

FACTOR =

and

SAME FACTOR

Only one factor is entered with FACTOR command and all components are modified by the same factor.

Notes:

1. Factors themselves are dimensionless but operate only on Molar Flowrate of the stream being modified.
2. Up to 150 component factors are allowed in this module.

Stream Manipulator Optional Command Details

Additional Modification Factors (Use Only With Multiply Factor)**SCF MOLe**

All component flowrates are multiplied by a SCF/MOL conversion factor in addition to being modified by the factors.

MOLe WEIght

All component flowrates are multiplied by their molecular weights in addition to being modified by the factors.

Stream Manipulator Command Summary

Modification Operators

ADD

SUBtract

Optional Commands

Modification Factors for MULTiply

SCF MOLe

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MULtiply
DIVide
HEAting VALue (no other calculation options)

Modification Factor(s)

FACTor =
or
FACTor =
and
SAMe FACTor

MOLe WEIght

Thermodynamics

HKEy=
KKEy=
DKEy=

Stream Manipulator Step by Step

Stream Manipulator STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier
Equipment number
Equipment name
Inlet stream
Outlet streams

STR

Assigned equipment flowsheet number
User choice - up to 16 characters
Unlimited in number
One or two; 1st copy of inlet; if two, 2nd is modified

Stream Manipulator STEP 2

Choose a way to modify stream components (enter ONE of the following)

Add factor to flowrate
Subtract factor from flowrate
Multiply flowrate by factor
Divide flowrate by factor
Calculate gross heating value (does not allow any other calculation options)

ADD
SUB
MUL
DIV
HEA VAL

Stream Manipulator STEP 3

Choose method for specifying factor(s). Modification factors (choose one of the following methods)

Enter a factor for each component
- Modification factors (separate factors with commas)
Enter same factor for all components
- Modification factor (one value)

FAC =
FAC =
and
SAM FAC

Stream modification options (use only with MULtiply factor)

Multiply factors by SCF/MOL conversion factor
Multiply components by their molecular weights

SCF MOL
MOL WEI

IF thermo is different from global (GENeral section) options THEN select

K-value option
Enthalpy option
Density option

KKE =
HKE =
DKE =

Stream Manipulator Examples

There are several sample flowsheets in "Chapter 42: Stream Manipulator Samples - c:\designii\samples\equipmnt\strman" of the DESIGN II for Windows Tutorial and Samples Guide.

Chapter 40: Tank

Tank is a module that calculates the dynamic behavior of feed, accumulations, and products from a constant volume tank. Temperature, pressure, and compositions will be calculated over a period of given time. Both pure components and mixed phases can be handled by the tank.

Tank Methodology

The initial time step calculates the initial amount of material in the tank. Subsequent time steps and additions from feed streams (if any), subtractions from product streams (if any), will calculate the resulting temperature, pressure and compositions of the tank. If there is a vent specified then the vent stream will allow vapor to bleed off to meet the vent pressure while maintaining adiabatic equilibrium.

The product streams can be started and/or stopped according to the user's time specifications. The liquid product streams will only run, if there is liquid in the tank and the vapor product streams will only run if there is vapor in the tank.

For example:

Product #1, start at 1 hr, stop at 3 hr

Product #2, start at 0 hr, stop at 4 hr

```
pr#1    <----->
pr#2 <----->
HR  +---+---+---+---+
    0   1   2   3   4
```

The product will only run if the start time is less than the current time and the stop time is zero or greater than the last time step value. Please also see [Calculation Options: Dynamic Simulation](#).

Tank Command Details

INITIAL CHARGE (Q units or FRA) = comp1, comp2, comp3, ...
Enter the initial charge for the tank.

INITIAL TEMPERATURE (T units) = value
Enter the initial temperature of the tank.

INITIAL PRESSURE (P units) = value
Enter the initial pressure of the tank.

VENT PRESSURE (P units) = value
Enter the vent pressure, if the tank is being vented.

PRODUCT FLOWRATE # (Q units / t units) = value
is 1, 2, 3, 4 or 5
Enter the product flowrate.

PRODUCT TYPE # = LIQUID or VAPOR
is 1, 2, 3, 4 or 5
Enter the product type (liquid or vapor).

START TIME # (t units) = value
Enter the starting time for products.

STOP TIME # (t units) = value
Enter the stopping time for products.

Tank Geometry

Following are commands to input tank geometry.

DIAMETER (L units) =
Enter the diameter of the tank.

HORIZONTAL
VERTICAL
SPHERICAL

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Enter one of the tank configuration. Default is VERTical.

LENGth (L units) =

Enter the length of the tank for horizontal or vertical tank configuration.

Initial **LIQuid HEIght** (L units) =

Enter the initial height of the liquid from the bottom of the tank.

Tank Command Summary

Specification Commands

INITIAL CHArge (Q units or FRA) = comp1, comp2, comp3, ...

INITIAL TEMPerature (T units) = value

INITIAL PREssure (P units) = value

VENT PREssure (P units) = value

PRODUCT FLOWrate # (Q units / t units) = value

is 1, 2, 3, 4 or 5

PRODUCT TYPE # = LIQuid or VAPor

is 1, 2, 3, 4 or 5

STArT TIME # (t units) = value

STOp TIME # (t units) = value

DIAMeter (L units) =

VERTical

SPHerical

LENGth (L units) =

Initial **LIQuid HEIght** (L units) =

Thermodynamic Commands

HKEy=

KKEy=

DKEy=

Tank Examples

Tank: Tank1.psd - Simulation of Heating a Tank

(From the DESIGN II Menu Bar, please select...File...Open... c:\designii\samples\equipmnt\tank\tank1.psd to simulate this problem)

Heating a tank to simulate a dynamic system.

AB123.

*Heating a Tank--To simulate a dynamic system

BASIS: 1 hr.

C- EQUIPMENT MODULES

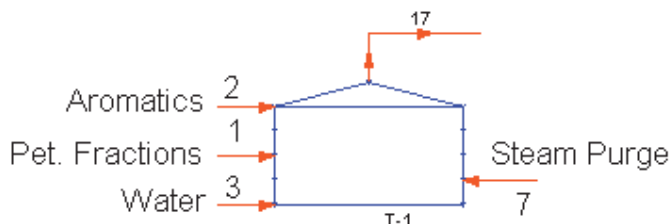
```
TANK 1 = T-1, 7,3,1,2,-17,  
VEN PRE (PSIA) = 14.696  
VER  
LEN (FT) = 6  
DIA (FT) = 20  
INI CHA (FRA) = 18*0,0.79,0.21,  
INI TEM (F) = 70  
INI PRE (PSIA) = 14.696
```

```
PRO TYP 1 = VAP  
STA TIM 1 (HR) = 0  
STO TIM 1 (HR) = 0  
PRO TYP 2 = VAP  
STA TIM 2 (HR) = 0  
STO TIM 2 (HR) = 0  
PRO TYP 3 = VAP  
STA TIM 3 (HR) = 0  
STO TIM 3 (HR) = 0  
PRO TYP 4 = VAP  
STA TIM 4 (HR) = 0  
STO TIM 4 (HR) = 0  
PRO TYP 5 = VAP  
STA TIM 5 (HR) = 0  
STO TIM 5 (HR) = 0
```

C- GENERAL SECTION

GENERAL

```
COMPONENTS = 62,1176,3111,3050,1140,3058,40,41,43,45,38,5003,10,8,11,12,13,14,  
46,47,100,101
```



```

NAM POS 1 = 'WATER'
NAM POS 2 = 'CCL2F2'
NAM POS 3 = '1,1,1-CL3 ETHANE'
NAM POS 4 = 'CL2HC-CH2CL'
NAM POS 5 = 'CL3 ETHYLENE'
NAM POS 6 = 'CL4 ETHYLENE'
NAM POS 7 = 'BENZENE'
NAM POS 8 = 'TOLUENE'
NAM POS 9 = 'M-XYLENE'
NAM POS 10 = 'ETHYLBENZENE'
NAM POS 11 = 'CYCLOHEXANE'
NAM POS 12 = 'NAPHTHALENE'
NAM POS 13 = 'N-HEXANE'
NAM POS 14 = 'N-PENTANE'
NAM POS 15 = 'N-HEPTANE'
NAM POS 16 = 'N-OCTANE'
NAM POS 17 = 'N-NONANE'
NAM POS 18 = 'N-DECANE'
NAM POS 19 = 'NITROGEN'
NAM POS 20 = 'OXYGEN'
NAM POS 21 = 'C7PLUS'
AMW 100 = 97
AMB (F) 100 = 187
API (API) 100 = 70
NAM POS 22 = 'C8PLUS'
AMW 101 = 107
AMB (F) 101 = 225
API (API) 101 = 61.6
C- Thermo Comments
  STDK
  STDH
  STDD
  DEN LIQ = STDD
  SUR TEN = STD
  AMB PRE (PSIA) = 14.696
  STA PRE (PSIA) = 14.696
  STA TEM (F) = 60
  NOR PRE (ATM) = 1
  AME UNI OUT
  MAX = 1
  CON TOL = 0.001
  FLO (LB/HR) 1 = 20*0,50,75,
  TP (F,PSIA) 1 = 70,14.7
  NAM STR 1 = Pet. Fractions
  FLO (LBMOL/HR) 2 = 0,1.5,20,1,18,27,90,102,75,5,3,40,2,15,10,7,14,5,2*0,
  TP (F,PSIA) 2 = 80,14.7
  NAM STR 2 = Aromatics
  FLO (GAL/DAY) 3 = 200,
  TP (F,PSIA) 3 = 80,14.7
  NAM STR 3 = Water
  FLO (LB/HR) 7 = 150,
  TP (F,PSIG) 7 = 600,150
  NAM STR 7 = Steam Purge
  NAM STR 17 = Tank Vent
END

```

Tank: Tank2.psd - Tank Vent with Nitrogen Purge

(From the DESIGN II Menu Bar, please select...File...Open... c:\designii\samples\equipmnt\tank\tank2.psd to simulate this problem)

Tank Vent with Nitrogen Purge

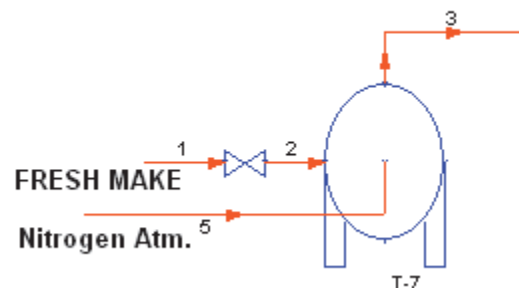
AB123.

*TANK Vent with Nitrogen Purge

C- EQUIPMENT MODULES

VAL 1 = FRESH MAKE, 1,-2,
PRE OUT (BAR) = 1.03

TANK 7 = T-7, 2,5,-3,
VEN PRE (BAR) = 1.03
SPH
DIA (M) = 32.961
HEA (KCAL/HR) = 26015000
INI CHA (LBMOL) =



Chapter 40

```
0,240000,129600,28800,12000,9600,7200,4800,
INI TEM(F) = -260
INI PRE (BAR) = 1.03
PRO TYP 1 = VAP
STA TIM 1 (HR) = 0
STO TIM 1 (HR) = 0
PRO TYP 2 = VAP
STA TIM 2 (HR) = 0
STO TIM 2 (HR) = 0
PRO TYP 3 = VAP
STA TIM 3 (HR) = 0
STO TIM 3 (HR) = 0
PRO TYP 4 = VAP
STA TIM 4 (HR) = 0
STO TIM 4 (HR) = 0
PRO TYP 5 = VAP
STA TIM 5 (HR) = 0
STO TIM 5 (HR) = 0
```

C- GENERAL SECTION

GENERAL

```
COMPONENTS = 46,2,3,4,5,6,7,8
NAM POS 1 = 'NITROGEN'
NAM POS 2 = 'METHANE'
NAM POS 3 = 'ETHANE'
NAM POS 4 = 'PROPANE'
NAM POS 5 = 'I-BUTANE'
NAM POS 6 = 'N-BUTANE'
NAM POS 7 = 'I-PENTANE'
NAM POS 8 = 'N-PENTANE'
```

C- Thermo Comments

```
APISOAVEK
APISOAVEH
STDD
DEN LIQ = STDD
SUR TEN = STD
AMB PRE (PSIA) = 14.696
STA PRE (PSIA) = 14.696
STA TEM(F) = 60
NOR PRE (ATM) = 1
AME UNI OUT
MAX = 20
CON TOL = 0.001
FLO (LBMOL/HR) 1 = 0,100,54,12,5,4,3,2,
TP (F,BAR) 1 = -260,1.05
NAM STR 1 = Strm 1
NAM STR 2 = Strm 2
NAM STR 3 = Vent Flow
FLO (LBMOL/HR) 5 = 1e-005,
TP (F,BAR) 5 = -100,1.05
NAM STR 5 = Nitrogen Atm.
TIME STEP (HR) = 1
TIME DUR (HR) = 24
```

END

Tank: Tank3.psd - Tank with Timed Multiple Product Draws

(From the DESIGN II Menu Bar, please select...File...Open... c:\designii\samples\equipmnt\tank\tank3.psd to simulate this problem)

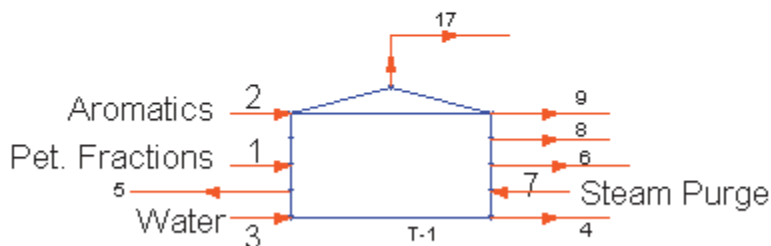
AB123.

*Tank with Timed Multiple
Product Draws

BASIS: 1 hr.

C- EQUIPMENT MODULES

```
TANK 1 = T-1, 7,3,1,2,-17,-4,-
9,-5,-6,-8,
VEN PRE (PSIA) = 14.696
VER
LEN (FT) = 6
DIA (FT) = 20
INI CHA (FRA) =
18*0,0.79,0.21,
INI TEM (F) = 70
INI PRE (PSIA) = 14.696
PRO FLO 1 (LBMOL/HR) = 4
PRO TYP 1 = LIQ
```




```

STA TIM 1(HR) = 0
STO TIM 1(HR) = 0
PRO FLO 2(MSCF/HR) = 9
PRO TYP 2 = VAP
STA TIM 2(MIN) = 5
STO TIM 2(HR) = 0
PRO FLO 3(GAL/MIN) = 5
PRO TYP 3 = LIQ
STA TIM 3(HR) = 0
STO TIM 3(HR) = 0
PRO FLO 4(LB/HR) = 6
PRO TYP 4 = VAP
STA TIM 4(HR) = 0
STO TIM 4(MIN) = 29.99
PRO FLO 5(BBL/DAY) = 8
PRO TYP 5 = LIQ
STA TIM 5(MIN) = 30
STO TIM 5(MIN) = 44

```

C- GENERAL SECTION

GENERAL

```

COMPONENTS = 62,1176,3111,3050,1140,3058,40,41,43,45,38,5003,10,8,11,12,13,14,
              46,47,100,101
NAM POS 1 = 'WATER'
NAM POS 2 = 'CCL2F2'
NAM POS 3 = '1,1,1-CL3 ETHANE'
NAM POS 4 = 'CL2HC-CH2CL'
NAM POS 5 = 'CL3 ETHYLENE'
NAM POS 6 = 'CL4 ETHYLENE'
NAM POS 7 = 'BENZENE'
NAM POS 8 = 'TOLUENE'
NAM POS 9 = 'M-XYLENE'
NAM POS 10 = 'ETHYLBENZENE'
NAM POS 11 = 'CYCLOHEXANE'
NAM POS 12 = 'NAPHTHALENE'
NAM POS 13 = 'N-HEXANE'
NAM POS 14 = 'N-PENTANE'
NAM POS 15 = 'N-HEPTANE'
NAM POS 16 = 'N-OCTANE'
NAM POS 17 = 'N-NONANE'
NAM POS 18 = 'N-DECANE'
NAM POS 19 = 'NITROGEN'
NAM POS 20 = 'OXYGEN'
NAM POS 21 = 'C7PLUS'
AMW 100 = 97
AMB (F) 100 = 187
API (API) 100 = 70
NAM POS 22 = 'C8PLUS'
AMW 101 = 107
AMB (F) 101 = 225
API (API) 101 = 61.6

```

C- Thermo Comments

```

STDK
STDH
STDD
DEN LIQ = STDD
SUR TEN = STD
AMB PRE(PSIA) = 14.696
STA PRE(PSIA) = 14.696
STA TEM(F) = 60
NOR PRE(ATM) = 1
AME UNI OUT
MAX = 1
CON TOL = 0.001
FLO(LB/HR)1 = 20*0,50,75,
TP (F,PSIA) 1 = 70,14.7
NAM STR 1 = Pet. Fractions
FLO(LBMOL/HR)2 = 0,1.5,20,1,18,27,90,102,75,5,3,40,2,15,10,7,14,5,2*0,
TP (F,PSIA) 2 = 80,14.7
NAM STR 2 = Aromatics
FLO(GAL/DAY)3 = 200,
TP (F,PSIA) 3 = 80,14.7
NAM STR 3 = Water
NAM STR 4 = Strm 4
NAM STR 5 = Strm 5
NAM STR 6 = Strm 6
FLO(LB/HR)7 = 150,
TP (F,PSIG) 7 = 600,150

```

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```
NAM STR 7 = Steam Purge  
NAM STR 8 = Strm 8  
NAM STR 9 = Strm 9  
NAM STR 17 = Tank Vent  
END
```

Tank References

1. "Plantwide Dynamic Simulators in Chemical Processing and Control (Chemical Industries)" by William Luyben.

Chapter 41: Valve

The VALve module is used for adiabatic (constant enthalpy) pressure reduction of a stream which can be vapor, liquid, or two-phase. If two or three outlet streams are coded, phase separation is performed. An essentially unlimited number of input streams can be coded; they will be adiabatically mixed to the lowest feed pressure.

Valve Features

The following features are also available when the VALve module is employed:

DEW and BUBble point pressure can be calculated. If only one outlet stream is coded, the phases are not separated. If two outlet streams are coded, the vapor phase is put into the first output, and the liquid into the second. Three-phase separations (water, gas, and hydrocarbons) can be performed if water has been declared immiscible in the GENeral section or you are using a K-value option that automatically treats water as immiscible. Vapor will be put in the first outlet stream, hydrocarbon liquid and soluble water will be placed in the second outlet, and "free water" plus soluble hydrocarbons will be placed in the third outlet stream. For the three-phase hydrocarbon-water system, you can also specify entrainment in the liquid phases.

You can request **sizing calculations** for the vessel performing the phase separation simply by using a few extra commands in your input. These results are intended for preliminary design work only and should not be used for detailed vessel design to A.S.M.E. code requirements (Reference 5). Simplifying assumptions have been made to facilitate preliminary sizing. DESIGN II can size any vertical or horizontal liquid-vapor separator, such as flash drums, reflux drums, accumulators, water knockout drums and inlet gas or compressor inlet separators.

Different types of separators may be sized in the same run using the sizing commands available for the VALve module. Physical properties of the vapor and liquid phases are obtained automatically from DESIGN II and do not have to be input by the user. These properties correspond to the vessel outlet conditions. An appropriate selection of K-values, enthalpy and density options should be made to obtain best results.

The program gives you a wide choice of sizing specifications and uses reasonable default values if you do not specify any. Vessel diameter, length and thickness are calculated and total weight of steel is estimated using a percentage allowance for supports and fittings. A scaled sketch is given for vertical vessels indicating the relative dimensions, liquid level and nozzle positions.

Valve Command Details

Valve: Pressure Specifications (choose only one)

PREssure **OUT** (P units) =

Enter desired outlet pressure. Default is inlet stream pressure.

DELta pressure (P units) =

Enter desired pressure change, to be subtracted from the inlet pressure. Default is 0.

Valve: Bubble and Dew Point Specifications (choose only one combination)

PREssure **OUT** is **DEW** point

The dew point pressure at the specified temperature is calculated and an adiabatic flash to the dew point pressure is performed.

and

TEMperature of **DEW** point (T units) =

Enter the dew point temperature at the specified pressure. Both commands must be used.

PREssure **OUT** is **BUB**ble point

The bubble point pressure at the specified temperature is calculated and an adiabatic flash to the bubble point pressure is performed.

and

TEMperature of **BUB**ble point (T units) =

Enter the bubble point temperature at the specified pressure. Both commands must be used.

Valve: Liquid CV Coefficient Specification

Liquid **CVC**oefficient (Q/P units) =

Enter desired liquid CV coefficient. This experimentally determined factor indicates the flow capacity of a liquid (incompressible flow) during non-choked, non-flashing flow through a valve with unit differential pressure. Only American units is allowed.

Default is none and has volume/pressure units (gpm/psi).

Valve: Non-Equilibrium Separation Commands

WATER ENTRAINED in OIL (units) =

Enter fractional value for water entrained in the oil phase.

OIL ENTRAINED in WATER (units) =

Enter fractional value for oil entrained in the water phase. The units options are MOLar, MASs, or VOLume. MOLar is the default option.

NOTE: IMM=62 must be specified in the GENeral section or you must be using a K-value option which automatically treats water as immiscible. Three outlet streams must be coded for the VALve module for this option. There are two options for calculating the solubility of water in the hydrocarbon phase. See THERMODYNAMIC/PROPERTY OPTIONS for details.

Valve: Separator Sizing Commands

The sizing calculation is performed if you specify either:

VERTical or **HORizontal**.

One of these is sufficient to obtain sizing results using default values. Sizing is also performed if any of the following commands are used, in which case the vessel is assumed to be VERTical unless otherwise specified. Reasonable default values are supplied by the program for unspecified commands.

K CONstant (L units/t units) =

Enter the K constant (velocity). Default is 0.35.

MIST ELIminator

Enter this command to specify that vessel has a 6 inch thick mist eliminator. Default option.

NO MIST eliminator

Enter this command to indicate that vessel does not have a mist eliminator.

ALLOWable stress (P units) =

Enter the allowable stress. Default is 15014.7 PSIA.

JOInt efficiency =

Enter the joint efficiency. Default is 1.0.

DESign pressure (P units) =

Enter the design pressure. Default is 10 percent higher than the inlet stream pressure.

CORrosion allowance (L units) =

Enter the corrosion allowance. Default is 0.125 inches. Remember that the default L unit is feet.

WEight PERcent allowance =

Enter the weight percent allowance. Default is 20.0.

RATio of MAJor to minor axes for head =

Enter the ratio of major to minor axes for the heads. Default is 2.0.

MINimum level NOZZle height (L units) =

Enter the minimum level nozzle height. Default is 1.5 feet.

Shell length is calculated from the length to diameter ratio for horizontal vessels. For vertical vessels, it is calculated from the sum of the high liquid level, minimum liquid to inlet height, minimum disengaging space and mist eliminator thickness (if present). You can override the calculated length using the following command:

LENGTH of SHEll (L units) =

Enter the length of the shell.

For a vertical vessel only, you can specify the following:

SURge time (t units) =

Enter the value for surge time. Default is 2 minutes.

MINimum DISengaging height =

Enter the minimum disengaging height. Default is 3 feet.

NOTE: The actual disengaging space selected is the diameter of the vessel if it is larger than the minimum disengaging height specified.

MINimum LIQuid to inlet height (L units) =

Enter the minimum distance between the inlet nozzle and the high liquid level. Default is 2 feet.

NOTE: The actual distance between the inlet nozzle and the high liquid level is at least one half the vessel diameter. It will be increased if necessary, to satisfy both the minimum liquid to inlet height and the total vessel length.

For a horizontal vessel only, you can specify the following:

LENGTH to DIAmeter ratio =

Enter the ratio of length to diameter. Default is 4.0. This ratio will then be used to calculate the length of the vessel.

MINimum VAPor height (L units) =

Enter the minimum vapor height. Default is 1.25 feet.

RESidence time (t units) =

Enter the residence time. Default is 5 minutes.

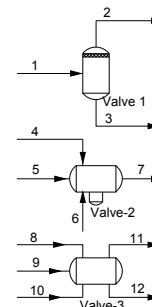
NOTE: The default time unit is HR. The residence time will be used to determine the normal minimum liquid level. This should include any additional settling time needed for the separation of two liquid phases.

BOOt DIAmeter (L units) =

Enter the boot diameter if you want to separate two liquid phases in the vessel. The second liquid phase will be contained in the boot. The program will calculate the size of the horizontal vessel required for the vapor and first liquid phase and the length of the boot for the second liquid phase. There is no default value for boot diameter. Weights reported for horizontal vessels include the combined weight for the vessel and boot.

Valve: Combined Equipment

The VALve module can be used for a pressure reduction and phase separation. The VALve module can be used for a mix of streams with a specified outlet pressure. Also, with the mix, a phase separation can be performed (2 or 3 outlet streams allowed).



Valve: Negative Pressure Drop or Pressure Increase

The pressure out of the VALve module can be specified higher than the feed pressure, which can be useful when you want to adjust the pressure of a stream. The outlet stream temperature will not be the same as would result from a compressor or pump calculation, as no work is being performed (constant enthalpy). For example, if you want to know the bubble point temperature of a stream at its storage pressure, you can adjust the pressure of the stream to the storage pressure with a VALve, and then use the HEAt EXChanger module or MULTiple FLAsh to calculate the bubble point temperature.

Valve: Use of Dew Point Specification

In a refrigeration cycle simulation, the refrigerant from the condenser must be lowered to the dew point pressure at which the refrigerant is to be used. An example of this usage is given in Refrigeration Cycle J-T Valve..

Valve: Use of Bubble Point Specification

In many natural gas simulations, the vapor pressure of the condensate at 100F is a product specification. Example 4, Bubble Point Pressure at Specified Temperature, shows how to use VALve and HEAt EXChanger modules to calculate this.

Valve Command Summary

Pressure Specifications

PREssure **OUT** (P units) =

DELta pressure (P units) =

Bubble and Dew Point Specifications

PREssure **OUT** is **DEW** point

and

TEMperature of **DEW** point (T units) =

PREssure **OUT** is **BUB**ble point

and

TEMperature of **BUB**ble point (T units) =

Liquid CV Coefficient Specification

Liquid **CVC**oefficient (Q/P units) =

Non-equilibrium Separation Commands

WATer **ENT**rained in **OIL** (units) =

OIL **ENT**rained in **WAT**er (units) =

Thermodynamic Commands

HKEy=

KKEy=

Separator Sizing Commands

VERTical or **HOR**izontal

K Constant (L units/t units) =

MISt **EL**iminator

NO MISt eliminator

ALLowable stress (P units) =

JOInt efficiency =

DESign pressure (P units) =

CORrosion allowance (L units) =

WEIght **PER**cent allowance =

RATio of **MAJ**or to minor axes for head =

MINimum level **NOZ**zle height (L units) =

LENgth of **SHE**ll (L units) =

SURge time (t units) =

MINimum **DIS**engaging height =

MINimum **LIQ**uid to inlet height (L units) =

LENgth to **DIA**meter ratio =

MINimum **VAP**or height (L units) =

RESidence time (t units) =

BOOt DIAmeter (L units) =

Chapter 41

DKEY=

Valve Step by Step

Valve STEP 1

Enter all the information below to uniquely define the module and its connections to the rest of the flowsheet.

Equipment name and connectivity (ALL are required).

Equipment module identifier

Equipment number

Equipment name

Inlet stream

Outlet streams

VAL

Assigned equipment flowsheet number

User choice - up to 16 characters

Unlimited in number

Up to three

Outlet stream coding specifications

- If only one outlet stream is coded, the phases are not separated
- If two outlet streams are coded, the vapor phase is put into the first output, and the liquid into the second
- For three-phase separations - water, gas and hydrocarbons, water must be declared immiscible in the GENERAL section or you must use a K-value option that automatically treats water as immiscible. Vapor will be put in the first outlet stream, hydrocarbon liquid and soluble water will be placed in the second outlet, and "free water" plus soluble hydrocarbons will be placed in the third outlet stream.

Valve STEP 2

Choose one of the pressure specifications listed below:

Outlet pressure

Pressure drop across the valve

PRE OUT (P units) =

DEL (P units) =

Valve STEP 3

Bubble and Dew Point Specifications (choose ONE of the following pairs)

Dew point specification

- Pressure out is dew point

- Dew point temperature

PRE OUT DEW

and

TEM DEW (T units) =

Bubble point specification

- Pressure out is bubble point

- Bubble point temperature

PRE OUT BUB

and

TEM BUB (T units) =

Liquid CV Coefficient Specification

Liquid CV Coefficient

CVC (Q/P units) =

OPTIONAL - Non-equilibrium Specifications (choose ANY of the following)

Water entrained in oil

Oil entrained in water

The units are MOLar, MASSs, or VOLume. Default is MOLar.

WAT ENT OIL (units) =

OIL ENT WAT (units) =

NOTE: IMM = 62 must be specified in the GENERAL section or you must be using a K-value option which automatically treats water as immiscible. Three outlet streams must be coded for the VALve module for this option. There are two options for calculating the solubility of water in the hydrocarbon phase. See *Thermodynamics: Water K-Values in Hydrocarbon Systems* for details.

Valve STEP 4

Separator Sizing

Vessel orientation

HORI or **VERT**

HORI or VERT is sufficient to obtain sizing results using default values. Entering any of the following commands will provide sizing results. The vessel is assumed to be VERTICAL unless otherwise specified. Reasonable default values are supplied by the program for unspecified commands.

K constant, velocity (default is 0.35)

Mist eliminator, six inch (default)

No mist eliminator

Allowable stress (default is 15014.7 PSIA)

Joint efficiency (default is 1.0)

Design pressure (default is 10% higher than inlet)

Corrosion allowance (default is 0.125 inches)

Weight percent allowance (default is 20.0)

Ratio of major to minor axes for heads (default is 2.0)

K CO (L units/t units) =

MIS ELI

NO MIS

ALL (P units) =

JOI =

DES (P units) =

COR (L units) =

WEI PER =

RAT MAJ =

Minimum level nozzle height (default is 1.5 feet)

MIN NOZ (L units) =

Shell length is calculated from the length to diameter ratio for horizontal vessels. For vertical vessels, it is calculated from the sum of the high liquid level, minimum liquid to inlet height, minimum disengaging space and mist eliminator thickness (if present). You can override the calculated length using the following command:

Length of the shell

LEN SHE (L units) =

For a vertical vessel only, you can specify the following:

Surge time (default is 2 minutes)

SUR (t units) =

Minimum disengaging height (default is 3 feet)

MIN DIS (L units) =

Minimum distance between the inlet nozzle and the high liquid level (default is 2 feet)

MIN LIQ (L units) =

For a horizontal vessel only, you can specify the following:

Ratio of length to diameter (default is 4.0)

LEN DIA =

Minimum vapor height (default is 1.25 feet)

MIN VAP (L units) =

Residence time (default is 5 minutes)

RES (t units) =

Boot diameter (no default)

BOO DIA (L units) =

IF thermo is different from global (GENeral section) options THEN select

K-value option

KKE =

Enthalpy option

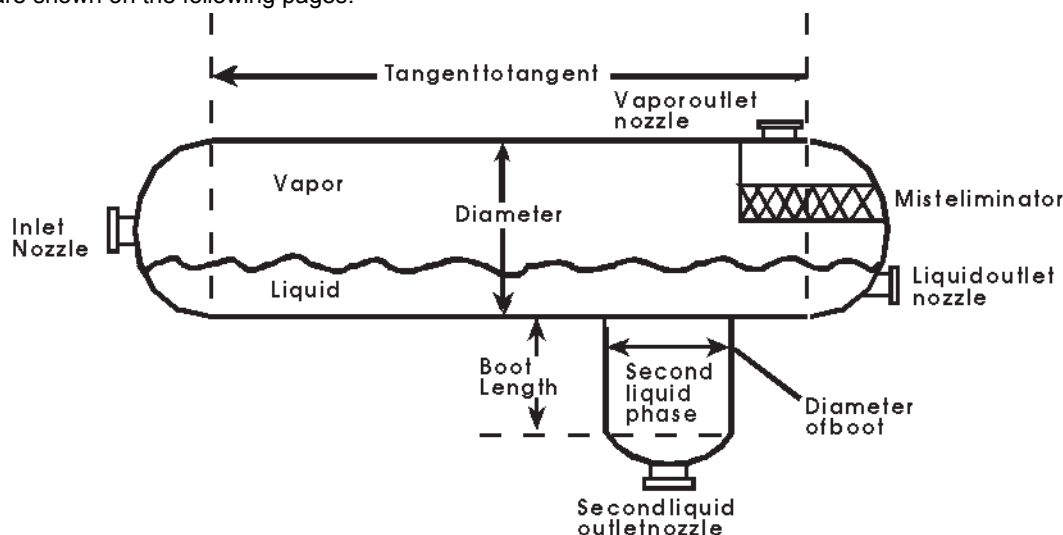
HKE =

Density option

DKE =

Valve Vessel Sizing

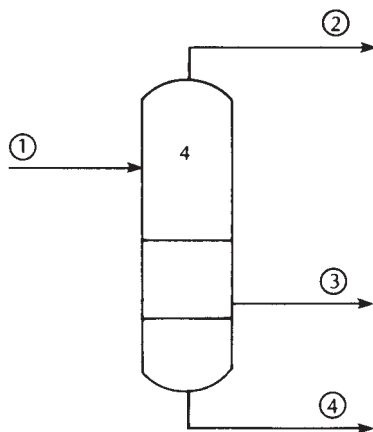
For vessel sizing guidelines, see ISOTHERMAL FLASH. Additional coding examples and the output for a horizontal separator with a boot are shown on the following pages.



Typical Horizontal Vessel with Optional Boot Examples

Valve Examples

There are several sample flowsheets in "Chapter 43: Valve Samples - c:\designii\samples\equipment\valve" of the DESIGN II for Windows Tutorial and Samples Guide.



```

VALve 4 = H2OD,1,-2,-3,-4,
GENeral,
    IMMiscible = 62
    
```

Method of Calculation

All properties of stream 1 are known. If there is any "free water" present, the vapor phase (stream 2) will be saturated. Stream 3 will contain liquid hydrocarbons and soluble water. Stream 4 will contain "free water" and soluble hydrocarbons. If CO₂, H₂S, and/or NH₃ are present the APISOUR correlation will be used to estimate their solubility in the water phase. Enthalpies and properties of the liquid streams will be recalculated.

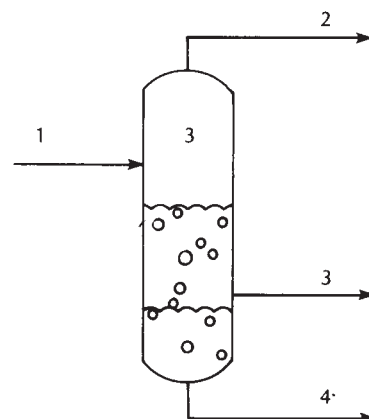
Valve: Entrainment of Oil and Water

```

VALve 3 = H2OD, 1,-2,-3,-4,
    OIL ENTrained in
WATER(VOL) = 0.0015,
    WATER ENTrained in OIL (VOL) = 0.02
GENeral,
    IMMiscible = 62
    
```

Method of Calculation

All properties of stream 1 are known. If there is any "free water" present, the vapor phase (stream 2) will be saturated. The liquid streams' composition will be calculated iteratively. Enthalpy and the physical properties of the liquid streams will be recalculated after the entertainment specifications are satisfied.

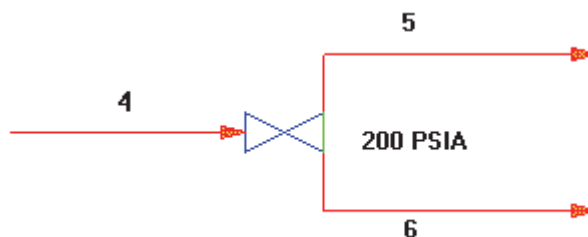


Valve: Typical Horizontal Vessel with Optional Boot Examples

Valve: Sour Water Stripper Reflux Accumulator

```

*SIZE STRIPPER REFLUX DRUM
VALve 1 = REFL, 1,-2,-3,
    HORIZontal,
    PREssure OUT (BAR) = 8,
    K Constant = 0.3,
    NO MIST eliminator,
    DESign pressure (BAR) = 10,
    MINimum VAPor space height (M) = 0.3,
GENeral,
    COMponents = 62,63,50,
    SOUR, YEN,
    FLOW 1 = 377.17, 35.313, 9.2437,
    TP (BAR) 1 = 195.6,23,
END
    
```

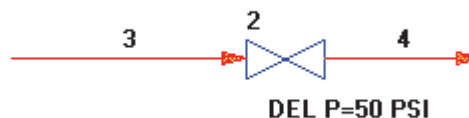


Valve: Horizontal 3 Phase Separator With Boot

```

*SIZE VESSEL AND BOOT
VALve 1 = 3 PHS, 1,-2,-3,-62,
    HORIZontal,
    BOOT DIAmeter(M) = .75, minimum
    RESidence time (MIN) = 6,
GENeral,
    COMponents= 2,3,4,5,6,7,8,10,11,12,100,62,
    AMB100 = 300,API 100 = 40, NAM100 = C8+,
    FLOW(KG/HR) 1 = 65493,6819,6000,1582,
        1055,982,782,909,518,268,817,
    TP (C,BAR) 1 = 38,60, IMM = 62,
    METric UNITS OUT, PREssure UNITS OUT = BAR,
END

```



A sample output for horizontal separator sizing example 2 is shown on the next page. Additional coding examples can be found in ISOTHERMAL FLASH, as well as a sample output for a vertical separator.

***** SEPARATOR SIZING RESULTS FOR HORIZONTAL SEPARATOR 1 *****

+++ WARNING: NO IMMISCIBLE PHASE EXISTS. BOOT IGNORED

VAPOR STREAM = 2 LIQUID1 STREAM = 3 LIQUID2 STREAM = 62

+++ WARNING : REQUIRED WALL THICKNESS 1.1239 IN. NOT AVAILABLE
IN 32.0 IN. NOMINAL PIPE. PLATE STEEL USED INSTEAD.

CONDITIONS

LIQUID 1	FLOW RATE	T-P	0.27281E-01	M3/MIN
LIQUID 2	FLOW RATE	T-P	0.00000E+00	M3/MIN
LIQUID TOT	FLOW RATE	T-P	0.27281E-01	M3/MIN
VAPOR	FLOW RATE	T-P	29.114	M3/MIN
TOTAL	FLOW RATE	T-P	29.142	M3/MIN
TEMPERATURE			38.000	DEG C
PRESSURE			60.000	BAR

PROPERTIES

DENSITY	LIQUID 1	627.32	KG/M3
DENSITY	LIQUID 2	0.00000E+00	KG/M3
DENSITY	VAPOR	49.125	KG/M3
Z-FACTOR	VAPOR	0.87849	

DESIGN PARAMETERS

LENGTH TO DIAMETER RATIO	DEFAULT	4.0000	
K CONSTANT	DEFAULT	0.10668	M/SEC
MIN LIQUID RESIDENCE TIME	SPEC	6.0000	MIN
MIN VAPOR SPACE HEIGHT	DEFAULT	0.38100	M
MIST ELIMINATOR	DEFAULT	0.15240	M
DESIGN PRESSURE	DEFAULT	66.000	BAR
ALLOWABLE STRESS	DEFAULT	1035.2	BAR
JOINT EFFICIENCY	DEFAULT	1.0000	
CORROSION ALLOWANCE (CA)	DEFAULT	0.31750E-02	M
WEIGHT PERCENT ALLOWANCE (WA)	DEFAULT	20.000	

RESULTS

MAX. DROPLET SETTLING VELOCITY	0.36599	M/SEC
ACTUAL VAPOR VELOCITY	1.8355	M/SEC
DIAMETER BASED ON SEPARATION	0.64385	M
SELECTED INTERNAL DIAMETER - PLATE STEEL	0.81280	M
LENGTH	3.6576	M
CORRESPONDING RESIDENCE TIME	35.444	MIN
NORMAL LIQUID LEVEL	0.40640	M
VAPOR SPACE HEIGHT	0.40640	M
ACTUAL PLATE THICKNESS	0.30163E-01	M
ACTUAL HEAD THICKNESS	0.30163E-01	M
MIN SHELL THICKNESS INCLUDING CA	0.29686E-01	M
MIN HEAD THICKNESS INCLUDING CA	0.28848E-01	M
APPROX WEIGHT OF STEEL VESSEL (EMPTY)	2433.6	KG
APPROX WEIGHT OF VESSEL (FULL)	3624.2	KG
APPROX TOTAL WEIGHT INCLUDING WA	4110.9	KG

NOZZLES (STD WALL)	INLET	VAP OUT	LIQ1 OUT	LIQ2 OUT
--------------------	-------	---------	----------	----------

Chapter 41

MINIMUM VELOCITY	10.39	10.44	2.922	0.0000E+00	M/SEC
ACTUAL VELOCITY	14.77	14.75	0.8002	0.0000E+00	M/SEC
MAXIMUM VELOCITY	17.31	17.40	4.871	0.0000E+00	M/SEC
NOMINAL DIAMETER	8.000	8.000	1.000	1.000	IN.

ESTIMATED SONIC VELOCITY IN VAPOR IS 398.0 M/SEC

NOTE : ONE OR MORE OF THESE NOZZLES DOES NOT MEET MIN AND MAX
VELOCITY SPECS BECAUSE SMALLEST NOZZLE SIZE IS 1 IN.

NOTE: INSULATION MAY BE NEEDED AS TEMPERATURE = 38.0 DEG C

CONSIDER USING A VERTICAL VESSEL SINCE LIQUID FLOW IS VERY SMALL.

THESE RESULTS ARE INTENDED FOR PRELIMINARY DESIGN WORK ONLY AND
SHOULD NOT BE USED FOR DETAILED VESSEL DESIGN TO A.S.M.E. CODE.

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