ChemShare News
1
1984

Announcing DESIGN II

The ChemShare Corporation • 1900 Lummus Tower • Houston, Texas 77056 • Phone: 713/627-8945 • Hot Line: 713/627-1760 • TWX: 910-881-2702

ChemShare news at a glance

Announcing DESIGN II

REFINE and DESIGN/2000 have been combined to create DESIGN II. This new ChemShare program is the most powerful process simulator available. (Story on page 3)

New product property specifications make it easy to improve the quality of one or more products without making numerous trial and error runs. (Story on page 5)

Heat exchange rating is available in DESIGN II. (Story on page 9)

New Features in DESIGN II

DESIGN II and DESIGN/2000 incorporate a number of new and improved features. Details and examples of these features are given in the following articles:

Lost work analysis (Story on page 12)

Material balance summary (Story on page 15)

Base pressure adjustment (Story on page 16)

Equipment sizing update (Story on page 16)

Metric/SI Units (Story on page 28)

Improved convergence technique (Story on page 29)

Amine treating (Story on page 29)

In-Line Fortran (Story on page 29)

New program ideas (Story on page 29)

Thermodynamics

Improved SELEXOL thermodynamic correlations are now available. (Story on page 31)

New UNIFAC groups have been added to ChemTran and DESIGN II. (Story on page 32)

MIXDAT

New LLE Database has been added to MIXDAT. (Story on page 33)

ChemTran

Several new features have been added to VLE and LLE data reduction. (Story on page 37)

General

Here's a unique opportunity to own source or object code for ChemTran and DESIGN II programs. (Story on page 43)

We are soliciting members for user groups for DESIGN II and ChemTran. (Information request on page 45)

ANNOUNCING DESIGN II

ChemShare has combined the DESIGN/2000 and REFINE programs to create DESIGN II. This is the most powerful process simulation software available. Some features not found in other simulators are:

1. Model any size flowsheet
2. Largest number of thermodynamic options
3. Largest pure component data base developed by a single source
4. Most flexible flash module
5. Largest number of end point specification options for products from crude distillation
6. units

   Separator sizing
7. Line sizing
8. Transmission line calculations
9. Prediction of CO2 solids formation on distillation trays or in streams
10. Most extensive plotting capability
11. Most powerful distillation column convergence algorithms

Every item listed is available in the DESIGN II program and therefore offers all the power of integrated software developed by one company. ChemShare's software is the most widely used and respected in the world. We continue to provide more capabilities via our on-going development program.

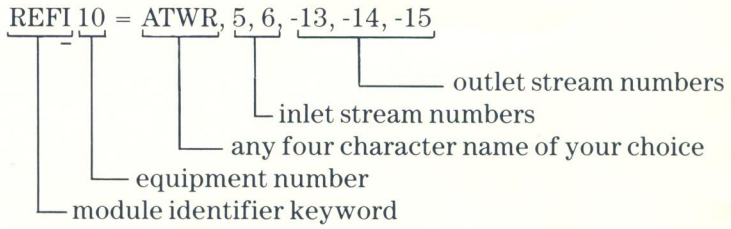
DESIGN II is now running on ChemShare's PR1ME 750s and will be installed on all other commercial systems during the regular updating cycle. Updates for IBM OS machines is schedules for mid-April.

DESIGN II is easy to use. It has the same simple keyword command approach you have used in DESIGN/2000 and REFINE. The following pages will show you how to convert REFINE input to DESIGN II input. A sample crude distillation flowsheet and the complete input file are also included.

Overview

All types of REFINE problems can now be run by the DESIGN II program. Most REFINE commands have been incorporated unchanged into the new program, but they are distributed among three sections of the DESIGN II input file. They are:

- REFIne module section - All REFINE commands which directly pertain to the column itself should be placed in the REFIne module input section. For each REFINE column in the run, you should have a separate REFIne module section. The module identifier is REFI. Equipment number, name, and inlet and outlet streams must be given as for any module. Steam feeds and water decants are not counted as streams. A typical REFI command is:



  Here are a few examples of REFINE commands that belong in this section:

  PUM REF
  STAGES = 8,2
  LOC FEE = 3,6
  LOC STE = 9,11
  STEAM(LB/HR) = 1500,800
  FIX TEM(C) = 120,1,1

- CRUde feed section - All REFINE commands which describe a feed stream should be placed in a separate section which begins with the CRU command. Some REFINE commands that belong here are:

  FEE(BBL/DAY)2 = 23400
  FEE ASTM2 = 225,410,450,500,620
  FEE VOL2 = 10,30,40,70,90
  FEE GRA2 = 27

- GENeral section - Global units options and thermo options should be placed here. For example:

  MET UNI OUT
  DAT TC KEY = 2

Command Changes

Although most of the REFINE commands have been incorporated directly into DESIGN II, there are some differences of which you should be aware. They are as follows:

- The TEM FEE and PRE FEE commands have been replaced by the DESIGN II TP command. You should enter a TP command in the CRUde section for each CRUde feed. For example:

  TP5 = 60,14.7

- The K-value, enthalpy, and density options are entered as keyword commands directly into the GENeral section. The REFINE commands DATA K KEY, DATA H KEY and DATA D KEY are no longer used. For example:

  ESSOTAB,API

- All feed commands within the CRUde section must have the stream number of the feed to which they pertain immediately before the equals sign, except CUT, TEM BRE, TEM INC, FEE COM GRA, and FEE COM MOL. For example:

  FEE GRA(SPG)1 = .85
  FEE VOL1 = 10,30,50,70,90
  CUT = 150,200,250,300,350,400,500,600

- A single run may now contain both distillation curve feeds and feeds which have already been broken down into pseudocomponents. If FEE COM MOL and FEE COM GRA are entered without stream numbers, they are assumed to apply to all feeds. If they are entered with a stream number, they apply only to that stream. For example:

  FEE(LB/HR)1 = 57000
  FEE VOL1 = 10,30,50,70,90
  FEE TBP1 = 250,300,420,550,790
  FEE GRA1 = 35
  FEE(BBL/HR)2 = 0,30,80,120,140,90,40
  FEE COM MOL2 = 99,128,163,206,256,378
  FEE COM GRA2 = 61,53,45,39,33,24
  CUT = 200,300,400,500,600,800
  GEN,COM = 62

Note that only one CUT command may be entered. If any feeds are present which have already been broken down into pseudo-components, then the CUT command must be entered.

- The following commands must now be entered separately for each CRUde feed stream to which they apply: FEE NAM, FEE BUL GRA, FEE BUL MOL, FEE BUL VIS SET, and FEE BUL PRO SET. They are no longer entered just once per run with a list of values after the equals sign. For example:

  FEE NAM1 = CRUDE
  FEE NAM2 = RECYCLE OIL
  FEE BUL GRA2 = 33.4

- Temporarily, if a CRUde feed section or a REFIne module is included in a run, water must be included in the COMponent list and it must be in the first position in the list. For example:

  GEN,COM = 62,2,3,4,5,6,8

- The default breakpoints for changing the petroleum fraction boiling point separation have been changed. Instead of 500°F and 700°F, they are now 600°F and 800°F. They may still be overridden with the TEM BRE command if required.

- The BLEnd and MIX commands no longer exist in the REFIne module. A MIXer module should be placed upstream of the REFIne module to combine feed streams. If you want the combined feed stream at a certain temperature (equivalent to the BLEnd command), use a HEAt EXChanger module with the TEM OUT command after the MIXer module and before the REFIne module. For example:

  MIX1 = BLND,1,2,-3
  HEA EXC2 = DUMX,3,-4,TEM OUT = 650
  REFI3 = TOWR,4,-5,-6,-7,-8

- In numbering STAges for a PUM PAR column, the condenser now counts as a stage.

- The FIX LIQ and FIX LIQ NET commands now use Hn instead of -n to indicate that the duty of the furnace on the nth feed should be varied. For example:

  FIX LIQ NET = 0,17,H1

- Continuation lines no longer must begin with four blanks.

- The REFINE FLAsh option no longer exists. Use the DESIGN II FLAsh, VALve, or MULtiFLAsh modules.

Thermodynamics

DESIGN II has all the K-value, enthalpy, and physical property correlations which were available in the DESIGN/2000 and REFINE programs. This gives you the largest number of thermodynamic options available in a simulation program. The default option for viscosity and thermal conductivity for DESIGN II is now the NBS81 technique (Ely-Hanley) unless your input file contains a CRUDE feed section, REFIne module or PETroleum STReam command. Correlations from the API Technical Data Book will then be used.

Water is automatically treated immiscibly in DESIGN II for the K-value options which are commonly used with hydrocarbon systems. The following options force water to be treated immiscibly:

APISOAVEK, BRAUNK, BWRK, BWRSK, CHAO, ESSOK, ESSOTAB, MOD ESSO, KVAL, RKK, SOAVEK, AND STDK (Chao-Seader with Grayson-Streed interactions).

These options force water to be treated miscibly:

APISOUR, MDEAK, SELK, and SOUR.

The remainder of the K-value options listed below default to treating water miscibly but you can specify IMM = 62 or GPAWAT.

IDEALK, PENK, RENON, TABK, UNIFACK, UNIQUACK, VAPPRE, WILSON.

If you want water treated miscibly for the first group of K-value options, you can enter a NOIMM command in the GENeral section of your input.

Output

If you have either a REFIne module or a CRUde feed description in your simulation, you will automatically get a detailed stream report for each stream which contains molar, mass and volume flows, mixture properties, and TBP, ASTM and gravity curves for each phase. To limit the number of stream reports which will be printed, you can enter the following command in the GENeral section:

PETroleum STReams = x, y, z

where x, y and z are the stream numbers in ascending order. You can delete this output entirely by specifying PETSTR = NONE. If you want the normal DESIGN II detailed stream print, simply add the following GENeral section command:

PRInt STReams = a,b,c

where a, b and c are appropriate stream numbers.

PRODUCT PROPERTY SPECIFICATIONS

You can use the PROduct SPEcification command in the REFIne module to optimize the properties of one or more products without having to make numerous trial and error runs. DESIGN II adjusts product rates to meet these specifications. The following product properties can be specified: 5% ASTM or TBP temperature, 95% ASTM or TBP temperature, ASTM or TBP initial boiling point, ASTM or TBP end points, ASTM gap, purity of a component or group of components, average molecular weight, average gravity, flash point and product rate. In addition, you may specify viscosity, pour point or other properties if you have entered the appropriate data using FEE VIS SET and FEE PRO SET commands.

The PRO SPE command is intended for tuning up product property specifications by making moderate adjustments in product rates. Before using a PRO SPE, you should have achieved a ballpark solution by changing the number of stages, duties or feed and draw locations. Do not use the PRO SPE command until you have a converged result for your ballpark solution. Then add your PRO SPE commands, update your temperature and molar flowrate guesses and rerun the simulation.

Example:
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.

Coding:
PRO SPE1 = 550,ASTM95,PROD3,PROD4

PRO SPE2 = 760,ASTM96,PROD4,PROD5

Example:
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)

Coding:
PRO SPE1 = 1.6,VISSET1,PROD5,PROD6

The format of the PRO SPE command is:

PRO SPE (units)j = A, B, C, D

where j is the specification number. All PRO SPE commands in the REFIne module input must be numbered sequentially beginning with 1.

A is the desired value of the property specified, in the units given by the (units) entry.

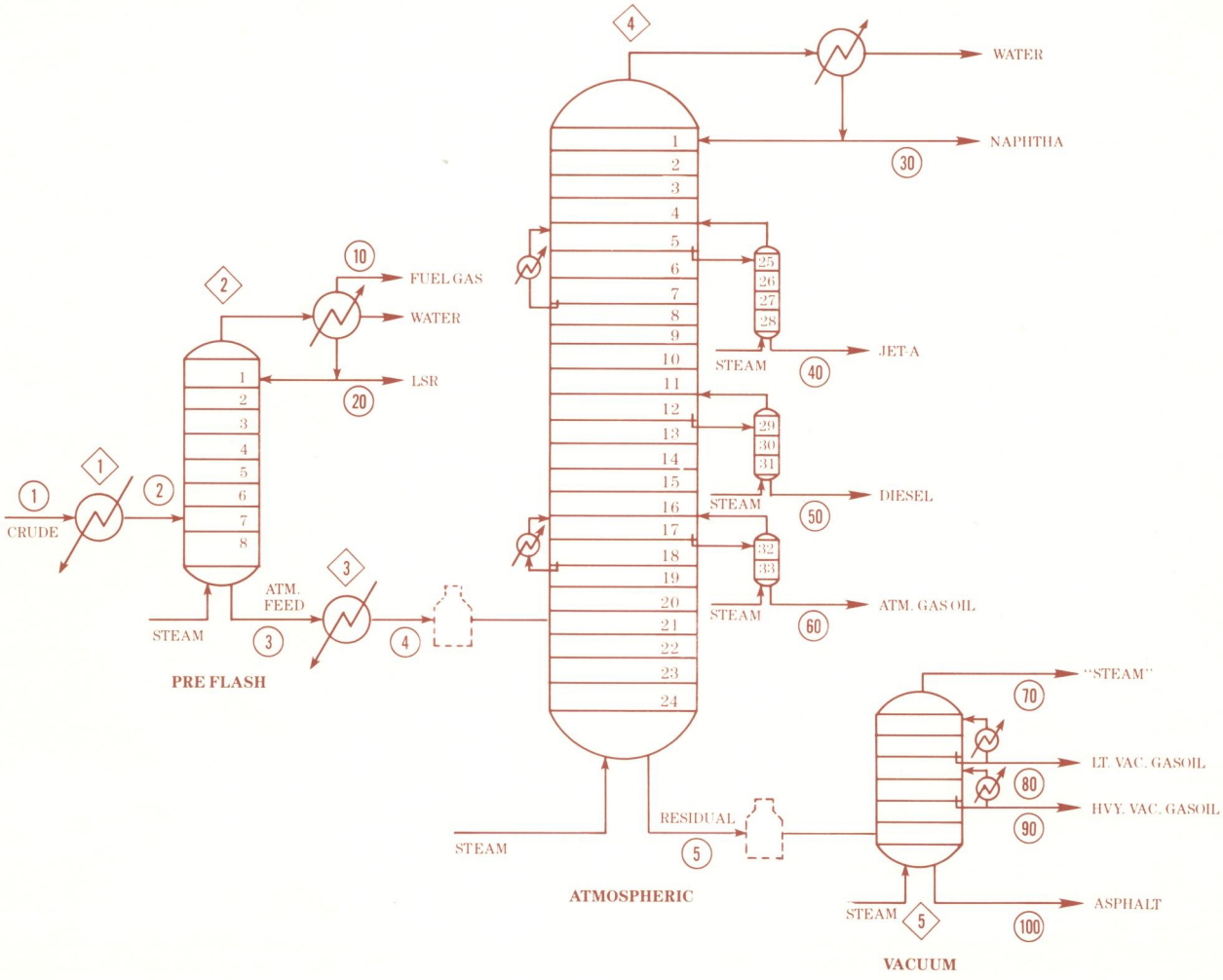
B is the name of the property specified. A complete list is given below.

C is the product to which the specification applies. This entry should be of the form PRODn, where n is the product number in top-to-bottom order.

D is the product whose rate will be varied to achieve the specification. The format is the same as for C.

Property Names

ASTM IBP	D-86 initial boiling point (0%)
ASTM 5PT	D-86 5% point
ASTM 95PT	D-86 95% point
ASTM EP	D-86 end point (100%)
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 (0%)
TBP 5PT	TBP 5% point
TBP 95PT	TBP 95% point
TBP EP	TBP end point (100%)
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 the mth components in the COMponent list.
AMW	average molecular weight
GRA	average gravity
FLA	flash point
FLO	mass or volume flow rate (you must specify volume or mass units for this option)
VIS SET n	viscosity from the nth viscosity data set
PRO SET n	property from the nth user supplied property data set
POUR	pour point from user provided pour point curves



Coding:

```
NN999.
*CRUDE FLOWSHEET - PREFLASH, ATMOSPHERIC, AND VACUUM
C-
C- PREHEAT FEED TO 450 F
C-
HEA EXC1 = PRHT, 1, -2, TEM OUT = 450, DELTA P = 10
C-
C- PREFLASH COLUMN
C-
REFI2 = PRFL,2,-10,-20,-3
PARTIAL, STAGES = 8, LOC FEE = 7
PRODUCTS(BBL/DAY) = 0,0,80000, PRO GUESS = 280,200,3900
PRE CON = 39.7, TEM CON = 160, PRE TOP = 41.7, DELTA P = 3
LOC STE = 8, PRE STE = 59, TEM STE = 400, STEAM(LB/HR) = 5000
TEM TOP GUESS = 340, TEM BOT GUESS = 450
PRODUCT NAMES = FUEL,LSR,ATM.FEED
REPORTS = 1
C-
C- ATMOSPHERIC FEED PREHEAT UP TO FEED FURNACE
C-
HEA EXC3 = INTR, 3, -4, TEM OUT = 625, DELTA P = 15
C-
C- ATMOSPHERIC TOWER
```

```
C-
REFI4 = ATM, 4, -30, -40, -50, -60, -5
TOTAL, STAGES = 24,4,3,2, LOC FEE = 21
PRODUCTS(BBL/DAY) = 0,35410, PRO GUESS = 575,1050
PRO STR(BBL/DAY) = 8165,16967,13290, PRO STR GUESS = 615,1050,625
PRE CON = 15.7, PRE TOP = 20.7, DELTA P = 4
TEM TOP GUESS = 360, TEM BOT GUESS = 620
LOC STE = 25,29,32,34, TEM STE = 4*400, PRE STE = 4*60
STEAM(LB/HR) = 12000,3300,1000,800
LOC PUMPAROUND = 7,5,13,12, HEAT PUM = 40E6,15E6
PRODUCT PUM(BBL/DAY) = 49000,11000, PRO PUM GUESS = 3600,700
LOC DRAWS = 5,12,17, LOC VAP RETURN = 5,12,17
FIX LIQUID(BBL/DAY) = 1500,20,H1
FIX GUESS = 50
PRODUCT SPEC1 = 625,ASTM95,PROD3,PROD4
PRODUCT NAMES = NAPHTHA,JET-A,DIESEL,ATM. GASOIL,ATM. RESID
REPORTS = 1
C-
C- VACUUM UNIT
C-
REFI5 = VTWR,5,-70,-80,-90,-100
PUM REF, STAGES = 6, LOC FEE = 5, LOC SID DRAW = 2,4
PRO(BBL/DAY) = 0,6200,18600,10600,PRO GUESS = 1.2,269,592,195
PRE TOP(MMHG) = 75, DELTA P(MMHG) = 30
LOC STE = 7, PRE STE = 59, TEM STE = 400, STEAM(LB/HR) = 20000
TEM TOP GUESS = 450, TEM BOT GUESS = 700
FIX TEM1 = 150,1,1,FIX LIQUID NET2 = 35,2,3
FIX LIQUID NET3 = 2,5,H1
LOC PUMPAROUNDS = 2,1,4,3,PRO PUM(BBL/DAY) = 20000,49000
HEA PUM = 14E6,54E6,PRO PUM GUE = 870,1560
PRO NAM = STEAM,LT VAC.GASOIL,HVY VAC.GASOIL,ASPHALT
C-
C- CRUDE FEED DESCRIPTION
C-
CRUDE FEED SECTION
FEED(BBL/DAY)1 = 100000
FEE GRA(API)1 = 150,95,65,45,40,38,33,30,25,20,15,10,5
FEE GRA VOL1 = 2,5,10,20,30,40,50,60,70,80,90,95,98
FEE VOLUME1 = 2,5,10,20,30,40,50,60,70,80,90,95,98,100
FEE TBP1 = -50,100,200,300,400,470,550,650,750,850,1100,1300,
1475,1670
FEE REAL1 = .1,.2,.5,.5,1,1.5,2.5
TEMP INCREMENT = 30,60,120,TEMP BREAKS = 500,900
TP1 = 215,59.7
C-
C- GENERAL INFORMATION
C-
GEN,COMPONENTS = 62,2,3,4,5,6,7,8
ESSOTAB,API
PETROLEUM STREAMS = 10,20,30,40,50,60,70,80,90,100
END
```

HEAT EXCHANGER RATING CALCULATIONS

DESIGN II version 1.0 and greater offers you a rating calculation for liquid-liquid counter-current heat exchangers. Simply add a RATe command to your heat exchanger input to request this calculation. There are additional commands which describe the geometry of the exchanger as well as material of construction. These commands are covered in separate documentation which we will be happy to send to you. A complete sample input is shown below with the rating results.

```
NN999.
* HEAT EXCHANGER RATING SAMPLE
FLA1 = FLSH,1,-2, -3
HEA EXC2 = G-GX,3,7,-4,-15,DEL TEM = -5,
RATE,SHELL TYPE IS AES
SHE DIA(FT) = 1.9,SHE FOU = 0.001
TUBE LAYOUT IS TRIAN
TUBE BWG = 18,TUBE NOT FINNED
TUBE MATERIAL = 2,TUBE LENGTH(FT) = 15
TUBE OUTSIDE DIA(FT) = 0.07
TUBE PITCH(FT) = 0.09
TUBE FOULING = 0.001,NUM TUB = 160
NUMBER SEALING STRIPS = 2
METHOD KERN,BAF SPA(FT) = 0.4
BAF CUT = 0.25
GEN,COM = 2,3,4,5,6,7,8,10,11,12,100,62
AMB100 = 300,API100 = 40,NAM100 = C8 +
FLO1 = 2*500,300,60,40,2*30,2*20,10,5,100
TP1 = 0,900
FLO(KG/HR)7 = 50,100,2000,100,53,10
TP(K,ATM)7 = 200,13.6
NO IMM
END
```

****** PROCESS RATING RESULTS FOR HEAT EXCHANGER 2 ******

HEAT EXCHANGER 2

G-GX

SIZE 23-180 TYPE AEL

		: SHELL SIDE	: TUBE SIDE
INLET TEMPERATURE	DEG F	: 0.0	: -99.7
OUTLET TEMPERATURE	DEG F	: -5.0	: -41.8
TOTAL FLUID	LB/HR	: 53686.	: 5099.3
VAPOR	(IN/OUT)	: 0./ 0.	: 0./ 0.
LIQUID	(IN/OUT)	: 53686./ 53686.	: 5099./ 5099.
INLET PRESSURE	PSIA	: 900.0	: 199.9
PRES DROP SPEC/CALC	PSIA	: 0.000 / 7.344	: 0.000 / 0.000
VELOCITY	FT/SEC	: 2.91	: 0.08
TOTAL HEAT EXCHANGED	BTU/HR	: -0.18947E 06	: 0.18947E 06
		:	:
PROPERTIES		:	:
		:	:
AVERAGE TEMPERATURE	DEG F	: -3.5	: -82.8
SP. GRAVITY	DEG API	: 232.7	: 163.5
MOLECULAR WEIGHT		: 33.	: 42.
VISCOSITY	CP	: 0.281	: 0.572
DENSITY	LB/FT3	: 30.345	: 36.699
SPECIFIC HEAT	BTU/LBMOL/R	: 23.450	: 27.398
THERMAL COND.	BTU/FT/HR/F	: 0.075	: 0.087
FOULING FACTOR	HR-FT2-F/BTU	: 0.0010	: 0.0010
		:	:

TOTAL HEAT EXCHANGED	BTU/HR	= 0.18947E 06
OVERALL U COEFF.	BTU/HR/FT2/F	= 21.881
LOG MEAN TEMPERATURE	DEG F	= 64.701
CORRECTION FACTOR		= 0.99
NO. OF SHELLS IN SERIES		= 1
NO. OF SHELL PARALLEL		= 1
TOTAL SURFACE AREA	FT2	= 527.79
EFFECTIVE SURFACE	FT2	= 135.46

METHOD FOR U & DELP CALCULATIONS IS KERN

CONSTRUCTION OF ONE SHELL

SHELL SIDE		TUBE SIDE	
I.D. IN	= 22.50	O.D. IN	= 0.875
BAF SPA IN	= 4.5	BWG	= 18
BAF CUT	= 0.25	LENGTH FT	= 15.00
NO. OF SEALING STRIPS	2	NO. OF PASSES	= 1
TUBE BUN DIA IN	= 0.00	NO. OF TUBES	= 160
BAF-SHEL CLE IN	= 0.00	PITCH TRI. IN	= 1.08

NEW FEATURES IN DESIGN II

We have been busy adding new capabilities and improving exisiting capabilities. Details and examples of these features are shown in the following pages. There is a complete set of documentation and/or sample problems for each of these new features which we will be happy to send to you. Please call or telex your sales representative at one of the following locations:

ChemShare Corporation
P. O. Box 1885
Houston, Texas 77001
Tel: (713) 627-8945
TWX: 910-881-2793

ChemShare Process Systems, Ltd.
Brook House, Church Street
Wilmslow, Cheshire SK9 1AT
Tel: (0625) 532113
Telex: 666905

Dr. A. H. Maute
Softec
Industriestrasse 54
D-7000 Stuttgart 80
West Germany
Tel: (0711) 7800495
Telex: 7255697

Am & Associates
311 Wassenaarseweg
2596 CV DEN Haag
Netherlands
Tel: (07028) 1359
Telex: 33574

Computer Engineering Applications
8th Floor, 14 Queens Road
Melbourne, Victoria 3004
Australia
Tel: (03) 2676299
Telex: 30333

Industrial & Offshore Computer
Services Pte Ltd.
P. O. Box 644
Telok Blangah West P. O.
Singapore 9110
Tel: 7795122
Telex: 27201

Seed H-K Ltd.
7/F Cheung Kong Building
661 Kings Road, North Point
Hong Kong
Telex: 780-60313

Soedarpo Service Bureau
J1 Let Jen S Parman 35
Jakarta, Barat
Indonesia
Telex: 45867

Taiwan Goodwinner Co. Ltd.
No. 8, 14 FL No 830 Hsin Yi Rd.
Sec. 2, Taipei
Taiwan, Republic of China
Telex: 26875

LOST WORK ANALYSIS

ChemShare has added a Lost Work analysis option to DESIGN II versions 1.0 and greater. This Lost Work analysis combines the First and Second Laws of Thermodynamics to evaluate the performance of a process.

The Lost Work concept, referred to as thermodynamic lost work, is different from the more commonly used concept of mechanical lost work. Mechanical lost work takes into account only the mechanical energy lost. Thermodynamic lost work represents the real loss which includes mechanical lost work and the reversible work required to offset the irreversible conversion. Therefore, thermodynamic lost work is a more practical representation of total loss in a process.

Thermodynamic lost work is defined as

$$LWt = LWm + LWrev$$

where LWt is total lost work,
LWm is mechanical lost work, and
LWrev is reversible work required to offset irreversible conversion of work.

In order to represent Lost Work effectively, a thermodynamic variable, availability function b, is used. It is defined as

$$b = h - T0\,s$$

where b is availability function in units of energy/mole,
h is enthalpy in units of energy/mole,
s is entropy in units of energy/mole, and
T0 is ambient temperature in degrees K or R.

The default value for T0 is 536.7°R (298°K).

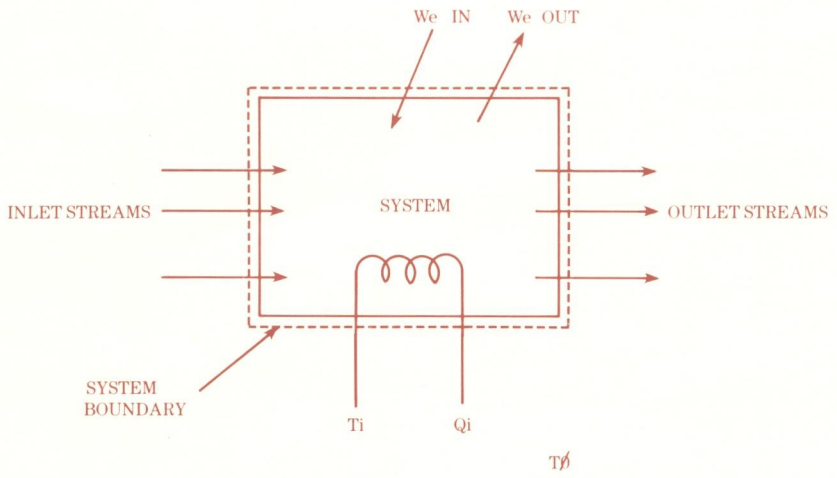
For a steady-state steady-flow process, Lost Work is shown as:

$$Wrev = \sum \dot{We} + L\dot{W}t = \sum_{j}^{nS} (bm)j + \sum_{i}^{nQ} (1 - T0/Ti)\,Qi$$

where $\sum$ We is the sum of all external work,

$\sum_{j}^{nS} (bm)j$ is the sum of availability function for all streams,

Ti is the exchange temperature, and
Qi is the amount of heat transferred across the system boundary. See Figure 1.



LOST WORK DIAGRAM

Figure 1

Lost Work is always positive for real processes and zero for an ideal reversible process. Strict sign convention for heat and work is required for the calculation.

The Lost Work analysis is effective in allowing you to evaluate process efficiency. When designing a new plant or optimizing existing processes, the Lost Work can be minimized to obtain higher thermodynamic efficiency. As high energy cost and waste heat recovery is becoming more important, the Lost Work analysis is a useful tool for process evaluation. For example, a Lost Work analysis can be used to compare the efficiency of two proposed separation schemes. In classical distillation, high temperature heat is added to the system in the reboiler and low temperature heat is removed in the condenser. The temperature driving force between the heat source and the heat sink is used to produce work in the form of separating the feed stream into its constituents. The difference between the theoretical maximum work which could be performed by the temperature driving force and the actual amount of separation work which is performed is the Lost Work. In distillation, one possible inefficiency which may be responsible for some Lost Work is a poor choice for feed location. Any time two streams of dissimilar composition are mixed, work is lost since it takes work to re-separate them. By varying the feed tray location and comparing the Lost Work reported by the program, you can optimize the feed tray location.

If you want a Lost Work analysis for your flowsheet calculation, simply enter a LOSt work command in the GENeral section of your input.

Exchange temperature can be overridden for individual equipments where Lost Work analysis is applicable. For process units such as multi-stage compressors, fired heaters, flashes with heat addition, heat exchangers, LNG exchangers, mixers and reactors, the command TEMperature EXChange (T units) = __ overrides the global exchange temperature. For equipments which require both heating and cooling fluids such as distillation and shortcut distillation columns, both the heating and cooling fluid temperatures can be set using the following commands:

TEMperature of HEAting fluid (T units) =
TEMperature of COOling fluid (T units) =

Lost Work analysis is not applied to certain equipment modules such as the controller, divider, isothermal flash, phase envelope, phase map, stream manipulator, multi-flash or add module. Lost Work for reactors is only calculated when heat and entropy of formation for all components are specified. This information is available automatically from the Pure Component Database for component ID numbers 1 through 98. For all other components, you should use the following GENeral section commands to enter this information:

HEAt of FORmation (H units/mole) i =
ENTropy of FORmation (S units) i =

where i is the component ID number.

Allowable entropy (S) units are:

BTU/LBMOL/R
CAL/GMOL/K
KCAL/KGMOL/K
J/GMOL/K

A sample of the Lost Work output is shown on the following page. Heat or mass flow into the system are reported as well as the Lost Work for each equipment which is printed in the last column of the table.

References:

de Nevers, Noel and Seader, J. D., "Mechanical lost work and thermodynamic efficiencies of processes", Presentation at the AIChE 86th National Meeting, Houston, Texas, April, 1979.

de Nevers, Noel and Seader, J. D., "Lost Work: A measure of thermodynamic efficiency", Energy, Vol. 5, p. 757 (1980).

LOST WORK ANALYSIS SUMMARY

EQUIPMENT NUMBER	TYPE	USER NAME	EXT. WORK BTU/HR	EXT. HEAT BTU/HR	EXCHANGE TEMP F	LOST WORK BTU/HR
1	HEAEXC	IGEX	-	-1.786E 07	-99.70	5.707E 06
2	FLA	SEPR	-	-	-	0.000
3	EXP	EXPD	3.199E 06	-	-	1.751E 06
4	CONT	FDFR	-	-	-	0.000
5	VAL	LCV1	-	-	-	8.971E 04
6	FLA	EOSP	-	-	-	0.000
7	DIS	DEMT				
	REBOILER		-	1.355E 06	250.00	-
	SIDE HEATER		-	8.000E 05	250.00	-
	TOTAL					9.777E 05
9	MIX	MIXR	-	-	-	4.034E 05
10	HEAEXC	GSEX	-	1.560E 07	250.00	8.150E 06
11	DIV	SPLT	-	-	-	0.000
12	COMPRE	BCMP	-3.198E 06	-	-	1.192E 06
13	PUM	PUMP	-3.286E 04	-	-	1.751E 05
15	PHA	ENVL	-	-	-	0.000
	TOTAL					1.8445E 07

*NOTE: IF LOST WORK IS NEGATIVE, REVIEW PARAMETERS FOR EQUIPMENT.

AVAILABILITY FUNCTION SUMMARY

STREAM NO	AVAIL. FUNC. BTU/HR	STREAM NO	AVAIL. FUNC. BTU/HR
1	2.25905E 07	10	7.68138E 05
2	2.56489E 07	11	2.93614E 05
3	2.47452E 07	13	1.94545E 07
4	9.03634E 05	14	1.51081E 07
5	1.97955E 07	15	1.50930E 07
6	8.08334E 05	16	1.70991E 07
7	1.97955E 07	17	1.51325E 05
8	1.90897E 07	20	15108.
9	7.05775E 05	70	8.98049E 05

DEFAULT OR SPECIFIED PARAMETERS:

AMBIENT TEMPERATURE:	77.00
HEATING FLUID TEMPERATURE:	250.00F
COOLING FLUID TEMPERATURE:	70.30F
REFRIGERANT TEMPERATURE:	-99.70F

MATERIAL BALANCE SUMMARY*

DESIGN II versions 1.0 or greater provides a new report which summarizes the material balance for each run. The total flows of all feed streams and product streams for the run are calculated. These flows (individual component basis and total) as well as differences between feed and products are reported. are reported.

The flows are reported on a molar basis except for cases which involve reactors—then the flows are reported on a weight basis. An example of a material balance summary is shown below. This report is included automatically in your output unless you have specified CHEck INPut or STOp= in the GENeral section.

*This feature is also available in DESIGN/2000 version 10.0.

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

COMPONENT NAME	FEED(S) LBMOL	PRODUCT(S) LBMOL	DIFFERENCE LBMOL	REL. ERROR
METHANE	5352.	5352.	0.2725	5.0909E-05
CO2	125.8	125.2	0.5616	4.4656E-03
H2S	31.32	31.26	5.8022E-02	1.8525E-03
WATER	9441.	9441.	-0.2168	-2.2964E-05
MONOETHANOLAMINE	0.0000	8.5466E-03	-8.5466E-03	-8.5466E 05
TOTAL FLOWRATE /HR	1.4950E 04	1.4949E 04	0.6660	4.4551E-05

BASE PRESSURE ADJUSTMENT*

The system base pressure can be changed from 14.696 PSIA to any other value so that the gas volume calculation is automatically corrected. This feature is useful for situations where a plant is to operate at elevations other than sea level.

The GENeral section command you use is

STAndard pressure (P units) =

This feature is available on DESIGN II versions 1.0 or greater.

EQUIPMENT SIZING UPDATE*

New sizing capabilities have been added to some of our equipment calculations in DESIGN II versions 1.0 or greater. An overview of these additions follows:

A. Glitsch column sizing

1. Specify diameter
2. Specify swage locations and diameters/ tray spacings

B. Separator sizing

1. Inlet scrubbers with no liquid flow
2. Three-phase separators such as water knockout drums (3 outlet streams allowed)
3. Estimation of sonic velocity for gas phase

C. Line sizing

Size lines based on maximum velocity by specifying a maximum sonic velocity fraction

D. Tranmission line modelling

An adiabatic model has been added

The following pages contain instructions for use of these new capabilities. In addition, portions of results are shown for some of these features.

*These features are also available in DESIGN/2000 version 10.0.

Glitsch tray sizing

The Glitsch short-cut technique has been improved so that you can now model existing columns with the diameter and tray spacing specified. The program then calculates the percent of flood on each tray. The new command for DIStillation and REFIne modules is as follows:

GLItsch DIAmeter (L units) =

Note: if you specify GLI DIA, you cannot specify GLItsch PERcent flood.

You can also model columns with different diameters in different sections by using the following commands:

GLItsch SWAge trays = j1, j2, . . .
GLItsch DIAmeters (L units) = ___, ___, ___, . . .

where j1 and j2 are the tray numbers immediately below the swage in the column. The number of values for diameters will always be one greater than the number of values for swages.

If you want to model a column with different tray spacings in different sections, you can use the following commands:

GLItsch SWAge trays = j1, j2, . . .
GLItsch SPAcing of trays (L units) = __, __, __, . . .

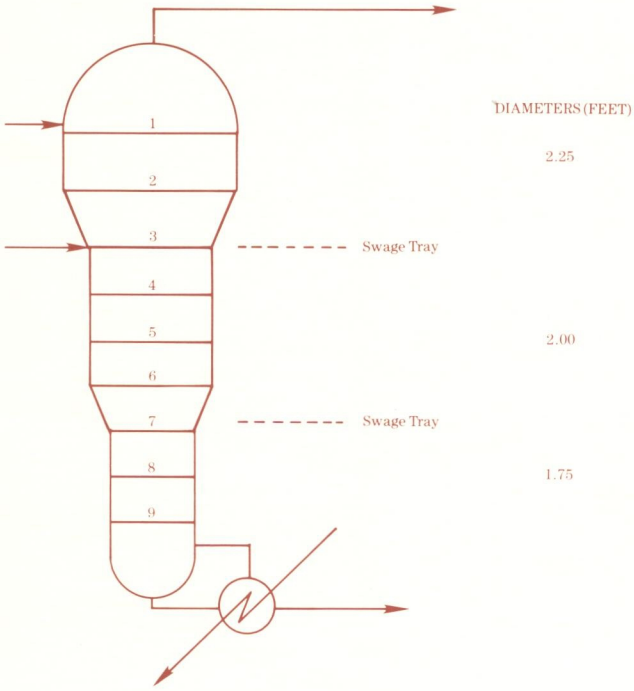
Once again, the number of values for tray spacing will be one greater than the number of values for swages. It is not necessary to specify diameter(s) in order to model different tray spacings.

A column which has both different diameter sections and tray spacings can be modelled by using all three commands together.

GLItsch SWAge trays = j1, j2, . . .
GLItsch DIAmeters (L units) = ___, ___, ___, . . .
GLItsch SPAcing of trays (L units) = __, __, __, . . .

The number of values entered for the diameter and tray spacing commands must be the same (and one greater than the number of values entered for swage trays command).

An example for a demethanizer is shown below.



GLITSCH SIZING DIAGRAM

This demethanizer has two swages resulting in three different column diameters. The input coding is:

```
NN999.
*DEMETHANIZER
DIS7=DEC1,9,6,-10,-11,ABS REB, TRA=9,
      LOC FEE=1,3,
      PRO=250,0,TEM TOP GUESS=-125,
      TEM BOT GUESS=50
      PRE TOP=190, DEL=6, LOC HEA=7,
      HEA=.8E6
      RAT BOT2,3=.025
      GLI DIA=2.5,2.25,2
      GLI SWA=3,7
GEN,COM=46,49,2,3,4,5,6,7,8,10
FLO9=2,24,73,36,6,5,.87,.47,.31
TP9=-135.7,200
FLO6=10,41,187,97,81,33,41,19,15,31
TP6=-102.4,200
SOAVEK,SOAVEH,COPED
END
```

The corresponding Glitsch results are shown below.

```
   GLITSCH SHORTCUT RESULTS FOR TRAY DIAMETER, PASSES AND PERCENT FLOOD
THE CORRELATION IS VALID FOR TRAY SPACINGS IN THE RANGE 12 - 48 IN.
AND PERCENT FLOOD IN THE RANGE 20 - 100.
                SYSTEM FACTOR =   1.00  (DEFAULT )
IT IS IMPORTANT TO USE THE CORRECT SYSTEM FACTOR (GLI SYS = ) FOR
FOAMING ON THE TRAY.   DEFAULT VALUE IS 1.0 WHICH IS APPROPRIATE
FOR NON-FOAMING, REGULAR SYSTEMS.   OTHER RECOMMENDED VALUES ARE :
OIL ABSORBERS, AMINE & GLYCOL REGENERATORS (MODERATE FOAMING) 0.85
AMINE AND GLYCOL ABSORBERS                 (HEAVY FOAMING)    0.73
MEK UNITS                                  (SEVERE FOAMING)   0.60
CAUSTIC REGENERATORS                       (FOAM-STABLE)      0.30
```

TRAY	SPECIFIED DIAMETER FT	LIQ FROM GAL/MIN	VAP TO FT3/SEC	CALC. NO. OF PASSES	CALC. PERCENT FLOOD	DEFAULT SPACING OF TRAYS IN.
0	MIXER	0.110E-02	1.35			
1	2.500	24.4	1.35	1.0	27.11	24.00
2	2.500	23.8	1.41	1.0	27.11	24.00
3	2.500	83.6	0.793	1.0	40.74	24.00
4	2.250	84.1	0.819	1.0	49.60	24.00
5	2.250	85.2	0.871	1.0	54.57	24.00
6	2.250	88.4	1.01	1.0	54.57	24.00
7	2.000	84.0	0.573	1.0	64.44	24.00
8	2.000	86.6	0.662	1.0	69.94	24.00
9	2.000	91.4	0.828	1.0	78.32	24.00
10	REBOILER	78.4	0.000			

Another example for review shows specifying the diameter for the column and using default values for all other sizing commands.

```
AB123.
*DEMETHANIZER
DIS7 = DEMT,9,6,-10,-11,TRA = 9,ABS REB,
LOC FEE = 1,3,PRO = 250,0
RAT BOT2,3 = .025,TEM TOP = -125,
TEM BOT = 50,PRE TOP = 190
DEL = 6,LOC HEA = 7,HEA = .8E6,
GLI DIA(IN) = 24
GEN,COM = 46,49,2,3,4,5,6,7,8,10
FLO9 = 2,24,73,79,36,6,5,.87,.47,.31
TP9 = -135.7,200
FLO6 = 10,41,187,97,81,33,41,19,15,31
TP6 = -102.4,200
SOAVEK,SOAVEH,COPED
METRIC UNITS OUT
END
```

The corresponding Glitsch results, using metric units, are shown below:

```
    GLITSCH SHORTCUT RESULTS FOR TRAY DIAMETER, PASSES AND PERCENT FLOOD
THE CORRELATION IS VALID FOR TRAY SPACINGS IN THE RANGE 12 - 48 IN.
AND PERCENT FLOOD IN THE RANGE 20 - 100.
                  SYSTEM FACTOR =   1.00  (DEFAULT )
IT IS IMPORTANT TO USE THE CORRECT SYSTEM FACTOR (GLI SYS = ) FOR
FOAMING ON THE TRAY.   DEFAULT VALUE IS 1.0 WHICH IS APPROPRIATE
FOR NON-FOAMING, REGULAR SYSTEMS.   OTHER RECOMMENDED VALUES ARE :
OIL ABSORBERS, AMINE & GLYCOL REGENERATORS (MODERATE FOAMING) 0.85
AMINE AND GLYCOL ABSORBERS                 (HEAVY FOAMING)    0.73
MEK UNITS                                  (SEVERE FOAMING)   0.60
CAUSTIC REGENERATORS                       (FOAM-STABLE)      0.30
```

TRAY	SPECIFIED DIAMETER M	LIQ FROM M3/HR	VAP TO M3/HR	CALC. NO. OF PASSES	CALC. PERCENT FLOOD	DEFAULT SPACING OF TRAYS M
0	MIXER	0.249E-03	138.			
1	0.610	5.54	138.	1.0	60.96	0.61
2	0.610	5.40	144.	1.0	60.96	0.61
3	0.610	19.0	80.9	1.0	64.44	0.61
4	0.610	19.1	83.5	1.0	68.00	0.61
5	0.610	19.3	88.8	1.0	69.94	0.61
6	0.610	20.1	103.	1.0	76.19	0.61
7	0.610	19.1	58.4	1.0	64.44	0.61
8	0.610	19.7	67.5	1.0	69.94	0.61
9	0.610	20.8	84.4	1.0	78.32	0.61
10	REBOILER	17.8	0.000			

SEPARATOR SIZING

Requests from users have resulted in several new features for the separator sizing capabilities. Sonic velocities for the gas phase are now reported automatically in the vessel output immediately after the nozzle table. You can now size gas scrubbers which normally have no liquid flow or three-phase separators such as water knockout drums (using FLAsh or VALve modules with two or three outlet streams coded).

An example and partial results for a gas scrubber and a water knockout drum are shown below. Notice that the program does not require any special commands to indicate which separator application you are modeling. You only need to indicate whether the vessel is vertical or horizontal.

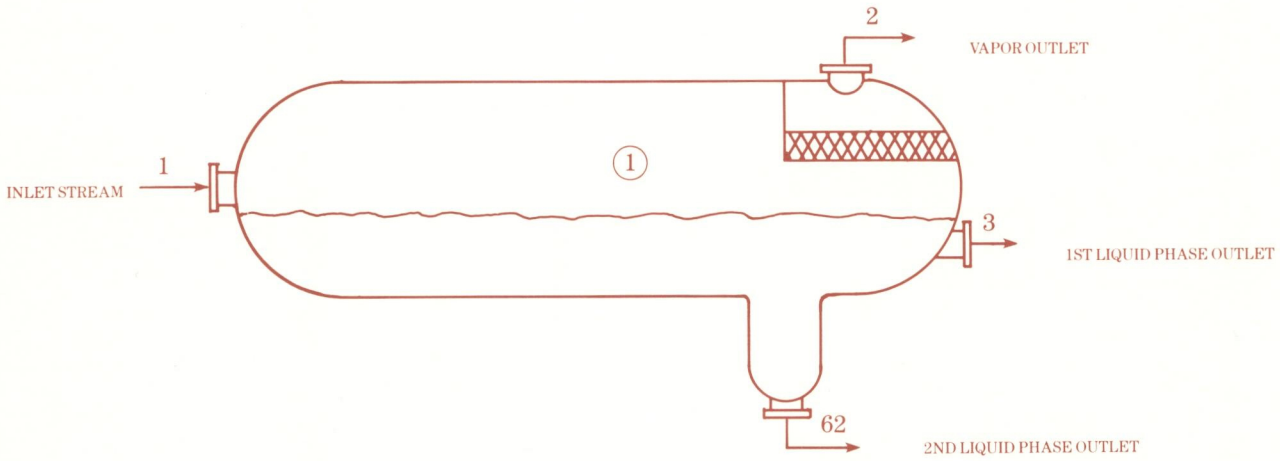
Example A. Compressor suction scrubber

Coding:

```
AB123.
* COMPRESSOR INLET SEPARATOR V101
FLASH DRUM1 = V101,1,-2,-3,VERTICAL
GEN,COM = 62,46,49,2,3,4,5,6,7,8,10
FLO(FRA)1 = .0145,.0005,.0075,.4450,.2255,.1950,.0225,.0585
            .0090,.0120,.0100
TP1 = 150,100
TOT FLO1 = 700
APISOAVEK,APISOAVEH,IMM = 62
END
```

```
      ****** SEPARATOR SIZING RESULTS FOR VERTICAL   SEPARATOR     1 *******
NOTE: NO LIQUID PRESENT AT THESE CONDITIONS.
      LIQUID DENSITY USED IS AT DEW POINT    67.4 F
       VAPOR STREAM =    2     LIQUID STREAM =    3
CONDITIONS
----------
LIQUID      FLOW RATE           T-P          0.00000       FT3/MIN
VAPOR       FLOW RATE           T-P           738.06       FT3/MIN
TOTAL       FLOW RATE           T-P           738.06       FT3/MIN
TEMPERATURE                                   150.00       DEG F
PRESSURE                                      100.00       PSIA
PROPERTIES
----------
DENSITY                         LIQUID         36.987      LB/FT3
DENSITY                         VAPOR         0.47750      LB/FT3
Z-FACTOR                        VAPOR         0.96701
RESULTS
-------
MAX. DROPLET SETTLING VELOCITY                 3.0605       FT/SEC
ACTUAL  VAPOR VELOCITY                         3.0373       FT/SEC
DIAMETER BASED ON SEPARATION                   2.2622       FT
SELECTED INTERNAL DIAMETER - PIPE              27.250       IN.
PIPE NOMINAL DIAMETER                          28.000       IN.
LENGTH                                         8.0000       FT
HIGH LIQUID LEVEL (HLL) HEIGHT                 1.5000       FT
HLL TO INLET HEIGHT                            3.0000       FT
DISENGAGING HEIGHT                             3.0000       FT
WALL THICKNESS (STD )                       0.31250E-01     FT
ACTUAL HEAD THICKNESS                       0.20833E-01     FT
MIN SHELL THICKNESS INCLUDING CA            0.17651E-01     FT
MIN HEAD  THICKNESS INCLUDING CA            0.17628E-01     FT
APPROX WEIGHT OF STEEL VESSEL(EMPTY)           926.20       LB
APPROX WEIGHT OF VESSEL (FULL)                 2124.6       LB
APPROX TOTAL WEIGHT INCLUDING WA               2309.8       LB


****** SEPARATOR SIZING RESULTS FOR VERTICAL   SEPARATOR     1 *******
NOZZLES (STD WALL)  INLET       VAP OUT      LIQ OUT
 .                    A             B            C
MINIMUM VELOCITY   86.829       86.829      0.00000      FT/SEC
ACTUAL  VELOCITY   139.14       139.14      0.00000      FT/SEC
MAXIMUM VELOCITY   144.72       144.72      0.00000      FT/SEC
NOMINAL DIAMETER   4.0000       4.0000       1.0000      IN.
     ESTIMATED SONIC VELOCITY IN VAPOR IS 1052.7 FT/SEC
```



Example B. Three-phase Separator (modeled as horizontal vessel with boot)

Coding:

```
NN999.
* WATER KNOCKOUT DRUM
FLA1 = FLASH, 1, -2, -3, -62, HORIZONTAL
BOOT DIA (M) = .75, MIN RESIDENCE TIME(MIN) = 6
GEN, COM=2,3,4,5,6,7,8,10,11,12,100,62,
AMB100=300,API100=40,NAM100=C8+
FLO(KG/HR)1=65493,6819,6000,1582,1055,
982,982,782,909,518,268,817
TP(C,BAR)1=38,60
MET UNI OUT, PRE UNI OUT=BAR
IMM=62
END
```

```
****** SEPARATOR SIZING RESULTS FOR HORIZONTAL SEPARATOR    1 *******
  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        0.17703E-01  M3/MIN
LIQUID  2  FLOW RATE          T-P        0.11033E-01  M3/MIN
LIQUID TOT FLOW RATE          T-P        0.28735E-01  M3/MIN
VAPOR      FLOW RATE          T-P         28.603      M3/MIN
TOTAL      FLOW RATE          T-P         28.632      M3/MIN
TEMPERATURE                               38.000      DEG C
PRESSURE                                  60.000      BAR
PROPERTIES
----------
DENSITY                      LIQUID 1     592.56      KG/M3
DENSITY                      LIQUID 2     992.78      KG/M3
DENSITY                      VAPOR        49.480      KG/M3
Z-FACTOR                     VAPOR       0.87630
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      65.999      BAR
BOOT DIAMETER FOR LIQUID 2               0.75000      M
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           0.40032      M/SEC
ACTUAL  VAPOR VELOCITY                    1.8376      M/SEC
DIAMETER BASED ON SEPARATION             0.61599      M
SELECTED INTERNAL DIAMETER - PLATE STEEL 0.81280      M
LENGTH                                    3.6576      M
CORRESPONDING RESIDENCE TIME              53.604      MIN
BOOT LENGTH                               1.3716      M
NORMAL LIQUID LEVEL                      0.40640      M
VAPOR SPACE HEIGHT                       0.40640      M
ACTUAL PLATE THICKNESS                   0.30162E-01  M
ACTUAL HEAD THICKNESS                    0.30162E-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)      3166.6      KG
APPROX WEIGHT OF VESSEL (FULL)            5091.5      KG
APPROX TOTAL WEIGHT INCLUDING WA          5724.8      KG
```

```
****** SEPARATOR SIZING RESULTS FOR HORIZONTAL SEPARATOR     1 *******
NOZZLES (STD WALL)   INLET      VAP OUT     LIQ1 OUT    LIQ2 OUT
MINIMUM VELOCITY     10.33       10.41        3.007       2.323      M/SEC
ACTUAL  VELOCITY     14.79       14.77       0.5291      0.3298      M/SEC
MAXIMUM VELOCITY     17.22       17.34        5.011       3.872      M/SEC
NOMINAL DIAMETER     8.000       8.000        1.000       1.000      IN.
     ESTIMATED SONIC VELOCITY IN VAPOR IS  362.3 M/SEC
 NOTE : ONE OR MORE OF THESE NOZZLES DOES NOT MEET MIN AND MAX
        VELOCITY SPECS BECAUSE SMALLEST NOZZLE SIZE IS 1 IN.
```

Line Sizing

Lines or nozzles can now be sized using a maximum velocity specification. The new command is:

MAXIMUM SONIC FRACTION =

The smallest diameter will be selected for each stream so that the fluid velocity does not exceed the specified fraction of sonic velocity. The estimated sonic velocity of the gas phase is automatically reported for vapor or two-phase streams. No sonic velocity calculation is performed if the stream is liquid.

This feature is useful for sizing flare headers for which you may have a limit on approach to sonic velocity.

You will notice in the following output that the 4 inch line (the smallest line) does not meet this specification while the others do.

Coding:

```
*FLARE GAS HEADER
FLASHDRUM19 = S306,16,-11,-44
VALVE20 = STACK,16,-12,-10,PRE OUT = 20
GEN,COM = 2,3,4
FLO16 = 10000,100,100
TP16 = 100,350
APISOAVEK
SIZELINES
USE STREAMS = 11
DIRECTION OF FLOW = HORI
LENGTH = 1000
MAX SON = .3
SIZE LINES
USE STREAMS = 12
DIRECTION OF FLOW = UP
LENGTH = 100
MAX SON = .5
END
```

********** LINE SIZING RESULTS FOR GAS STREAM 11 **********
LINE IS ISOTHERMAL AND HORIZONTAL
METHODS USED : FRICTION DELTA P DARCY FRICTION FACTOR MOODY ELEVATION DELTA P PHASE DENSITY

VAPOR FLOW RATE	LB/HR	0.1678E 06	
TEMPERATURE	DEG F	100.0	
INLET PRESSURE	PSIA	350.0	
MAX SONIC FRACTION		0.3000	SPECIFIED
LINE LENGTH	FT	1000.	SPECIFIED
ELEVATION	FT	0.0000	DEFAULT
PIPE WALL CODE		STD	DEFAULT
PIPE ROUGHNESS	FT	0.1500E-03	DEFAULT
DENSITY (VAPOR)	LB/FT3	0.9974	
MOLECULAR WEIGHT (VAPOR)		16.46	
VISCOSITY (VAPOR)	CP	0.1204E-01	
Z-FACTOR(AT INLET PRESSURE)		0.9614	
SONIC VELOCITY		1451. FT/SEC	

* *

		LARGER	TARGET	SMALLER
NOMINAL DIAMETER	IN.	6.000	5.000	4.000
INTERNAL DIAMETER	IN.	6.065	5.047	4.026
DELTA P (FRICTION)	PSI	173.1	450.6	1464.
DELTA P (ELEVATION)	PSI	0.0000	0.0000	0.0000
DELTA P (TOTAL)	PSI	173.1	450.6	1464.
PRESSURE DROP/100FT	PSI	17.31	45.06	146.4
MEETS VELOCITY SPEC		YES	YES	NO
OUTLET PRESSURE	PSIA	176.9	0.0000	0.0000
FLUID VELOCITY	FT/SEC	233.0	336.5	528.8
TRANSITION REYNOLDS NUMBER		0.2886E 06	0.2355E 06	0.1833E 06
REYNOLDS NUMBER		0.1451E 08	0.1744E 08	0.2186E 08
FLOW REGIME		TURBULENT	TURBULENT	TURBULENT
FRICTION FACTOR		0.1497E-01	0.1555E-01	0.1631E-01

********** LINE SIZING RESULTS FOR GAS STREAM 12 **********
LINE IS ISOTHERMAL AND VERTICAL (UP)
METHODS USED : FRICTION DELTA P FRICTION FACTOR ELEVATION DELTA P
DARCY MOODY PHASE DENSITY

VAPOR FLOW RATE	LB/HR	0.1678E 06	
TEMPERATURE	DEG F	82.95	
INLET PRESSURE	PSIA	20.00	
MAX SONIC FRACTION		0.5000	SPECIFIED
LINE LENGTH	FT	100.0	SPECIFIED
ELEVATION	FT	100.0	DEFAULT
PIPE WALL CODE		STD	DEFAULT
PIPE ROUGHNESS	FT	0.1500E-03	DEFAULT
DENSITY (VAPOR)	LB/FT3	0.5664E-01	
MOLECULAR WEIGHT (VAPOR)		16.46	
VISCOSITY (VAPOR)	CP	0.1133E-01	
Z-FACTOR(AT INLET PRESSURE)		0.9978	
SONIC VELOCITY		1453. FT/SEC	

* *

		LARGER	TARGET	SMALLER
NOMINAL DIAMETER	IN.	18.00	16.00	14.00
INTERNAL DIAMETER	IN.	17.25	15.25	13.25
DELTA P (FRICTION)	PSI	1.357	2.559	5.302
DELTA P (ELEVATION)	PSI	0.3934E-01	0.3934E-01	0.3934E-01
DELTA P (TOTAL)	PSI	1.396	2.598	5.341
MEETS VELOCITY SPEC		YES	YES	NO
OUTLET PRESSURE	PSIA	18.60	17.40	14.66
FLUID VELOCITY	FT/SEC	507.2	648.9	859.6
TRANSITION REYNOLDS NUMBER		0.9118E 06	0.7966E 06	0.6827E 06
REYNOLDS NUMBER		0.5426E 07	0.6137E 07	0.7064E 07
FLOW REGIME		TURBULENT	TURBULENT	TURBULENT
FRICTION FACTOR		0.1240E-01	0.1263E-01	0.1296E-01

Pipeline Modeling

You can now choose between isothermal or adiabatic calculations for the LINE module. Add the following command to your LINE module input if you want an adiabatic calculation:

ADIabatic

The ADIabatic command allows the program to take into account effects such as flashing or retrograde condensation due to pressure drop in the LINE. The default calculation option is isothermal.

A LINE with significant pressure drop should be modeled in several increments as an adiabatic flash will be performed for each increment you specify in the LENgth command. An example of an adiabatic offshore LINE with two-phase flow is shown below. This case also shows how to model an elevation profile along the sea bed.

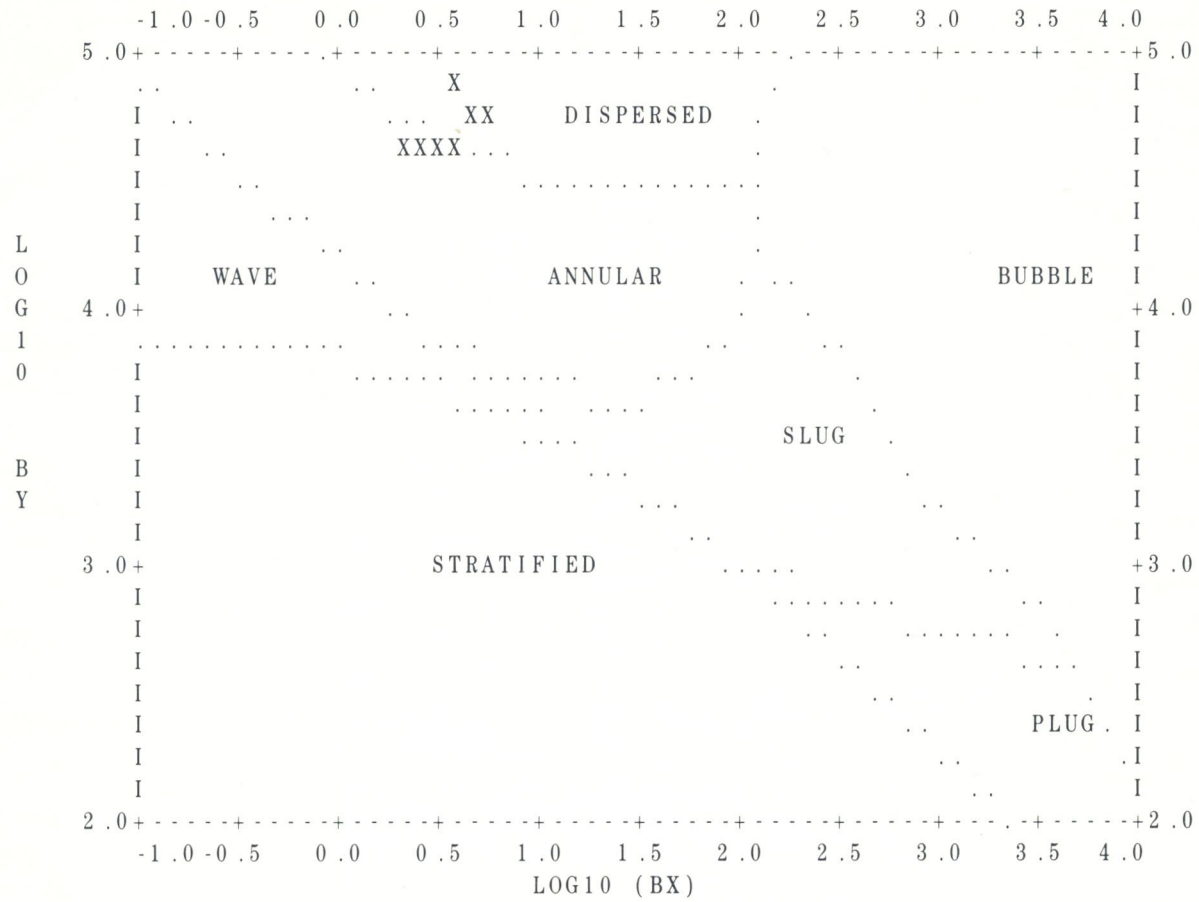
```
NN999.
*ADIABATIC TRANSMISSION LINE
LINE1=TRX,1,-2, NOMINAL DIAMETER(IN)=24
        LENGTH(MILES)=10*10, ADIA
        ELEVATION(FT)=10,5,-2,6,3,4,5,7,2,8
GEN,COM=46,49,2,3,4,5,6,8,10,11,12,62
FLO(FRA)1=.0120,.0120,.7114,.1099,.0934,.0386,
          .0096,.0022,.0007,.0002,.01
TOTAL FLOW(MMSCF/DAY)1=400
TP1=120,1600
PENGK,PENGH,BIN PAR=PENG1
BWRSD,TRANS=NBS81
END
```

```
                RESULTS OF LINE     1       -       WET GAS FLOW
                INLET STREAM(S)     1
                OUTLET STREAM(S)    2
                LINE CHARACTERISTICS: HORIZONTAL
                                      ADIABATIC
                ELEVATIONS ARE REPORTED RELATIVE TO INLET NODE.

VAPOR FLOW RATE    SCF/HR     0.1642E 08  LIQUID FLOW RATE  GAL/HR     0.2720E 04
PIPE ROUGHNESS     FT         0.1500E-03  PIPE EFFICIENCY FACTOR       0.1000E 01
NOMINAL DIAMETER   INCHES    24.000       PIPE WALL THICKNESS CODE     STD
INTERNAL DIAMETER  INCHES    23.250
METHODS FOR: FRICTION DELTA P     FRICTION FACTOR      ELEVATION DELTA P
             LOCKHART-MARTINELLI  MOODY                PHASE DENSITY
METHODS FOR: LIQUID HOLDUP        FLOW REGIME
             HUGHMARK             BAKER

PRESSURE DROPS (DELP) ARE FROM THIS NODE TO NEXT NODE.

LINE     LENGTH    ELEV.   TEMP.  DELP-FRIC  DELP-ELEV  PRESS.  VELOC.  LIQUID   FLOW
NODE       FT        FT    DEG F     PSI        PSI      PSIA   FT/SEC  HOLDUP  REGIME
  1         0.0      0.0   120.0     37.40      0.73   1600.00    11.7  0.1018   ANNU
  2     52800.0     10.0   118.5     40.34      0.36   1561.87    12.0  0.1073   ANNU
  3    105600.0     15.0   116.9     69.93     -0.14   1521.17    12.3  0.1118   DISP
  4    158400.0     13.0   114.1     81.17      0.42   1451.39    12.9  0.1166   DISP
  5    211200.0     19.0   110.6     92.54      0.20   1369.80    13.7  0.1198   DISP
  6    264000.0     22.0   106.4    104.62      0.26   1277.06    14.7  0.1211   DISP
  7    316800.0     26.0   101.4    117.86      0.31   1172.18    16.1  0.1203   DISP
  8    369600.0     31.0    95.3    133.75      0.40   1054.01    18.0  0.1174   DISP
  9    422400.0     38.0    88.0    153.91      0.10    919.85    20.7  0.1118   DISP
 10    475200.0     40.0    78.7    182.19      0.37    765.84    25.2  0.1023   DISP
 11    528000.0     48.0    66.2                        583.28    33.8  0.0864   DISP
       ESTIMATED SONIC VELOCITY IN GAS PHASE
         =    1189.2 FT/SEC    AT INLET CONDITIONS.
         =    1116.0 FT/SEC    AT OUTLET CONDITIONS.
```


******* BAKER TWO-PHASE FLOW REGIME MAP FOR LINE 1 *******
-1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0
5.0
4.0
3.0
2.0
WAVE
ANNULAR
BUBBLE
DISPERSED
STRATIFIED
SLUG
PLUG
LOG10 (BY)
LOG10 (BX)

METRIC/SI UNITS*

Input and output units control is much easier and requires less typing in DESIGN II versions 1.0. Simply enter either of the following commands in the GENeral section of your input: the GENeral section of your input:

METric UNIts
SI UNIts

The program will use the appropriate units for both the input and output sections of your simulation. You can still enter units options for specific keyword commands as shown in the User Guide. You can use any combination of the following new commands to reset the input/output units for a specific category:

QUAntity UNIts = (molar flow only)
TEMperature UNIts =
PREssure UNIts =
ENThalpy UNIts =
TIMe UNIts =
LENgth UNIts =

Coding:

```
NN999.
*EXPANDER PLANT EXAMPLE
HEAEXC1 = CHIL,1,-2,TEM OUT(C) = -40,
DEL(BAR) = .69
FLA2 = CSEP,2,-3,-4,
EXP3 = E33,3,-5,-6,PRE OUT(BAR) = 20.684
GEN,COM = 2,3,4
FLO(KGMOL/HR)1 = 1000,200,100
TP(C,BAR)1 = 37.784,55.157
APISOAVEK,APISOAVEH
MET UNI OUT,PRE UNI OUT = BAR
END
```

The input shown below is equivalent to the sample file above, but requires less typing because the MET UNI and PRE UNI commands are used.

```
NN999.
*EXPANDER PLANT EXAMPLE
HEAEXC1 = CHIL,1,-2,TEM OUT = -40,DEL = .69
FLA2 = CSEP,2,-3,-4
EXP3 = E33,3,-5,-6,PRE OUT = 20.684
GEN,COM = 2,3,4
FLO1 = 1000,200,100
TP1 = 37.784,55.157
APISOAVEK,APISOAVEH
MET UNI,PRE UNI = BAR
END
```

A table of the standard unit options for each category of each system is given on the following page.

*This feature is also available in DESIGN/2000 version 10.0.

Unit Options by System

	Default	Metric	SI
Quantity	LBMOL	KGMOL	KGMOL
Pressure	PSIA	KG/CM2	KPA
Temperature	F	C	K
Enthalpy	BTU	KCAL	KJ
Length	FT	M	M
Power	HP	METRIC HP	WATTS
Time	HR	HR	SEC
Heat transfer	BTU/HR/FT2/F	KCAL/HR/M2/C	KJ/SEC/M2/K
Gravity	API*	SPG	SPG
Rotational speed	RPM	RPM	RPS

*Input only; results will report specific gravity or density.

IMPROVED CONVERGENCE TECHNIQUE

You may have noticed that your distillation columns are converging more quickly or with less effort on your part. Dr. Gary Fisher has made some improvements in the distillation algorithm for highly non-ideal systems such as amine or sour water systems where small changes in temperature can cause large changes in composition.

AMINE TREATING

Do you have a problem no one has been able to solve? Give our amine capabilities a try. Two large E&C companies recently brought their problems to ChemShare after little success elsewhere. Both cases tested different "limits" of most amine correlations. Our program came through with flying colors. We matched actual plant data very closely. Temperatures matched within 2-6 °F (2-3%), duties matched within 2-5% and sweet gas compositions for CO_2 and H_2S ranged from 2-4%.

FIRST AND BETTER

ChemShare has always striven to bring you better features and to give them to you first. For example: **Did you know**

that ChemShare has had an automatic sequence calculation sequence algorithm in DESIGN/2000 for 15 years?

that the CONTroller module for passing information between modules or solving setpoint calculations has been available for over 10 years?

that In-Line Fortran is now available on PR1ME, DEC and IBM systems?

In-Line Fortran allows you to write your own Fortran subroutines for special calculations or to modify existing calculations in modules which are currently available in DESIGN II. And we're not through yet. Watch future newsletters for additional capabilities.

NEW PROGRAM IDEAS

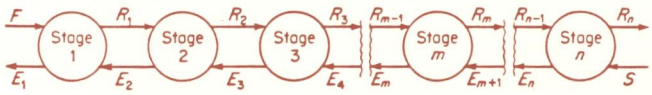
We've said it once, we'll say it again—our programs are not cast in concrete. We bring you new features or improvements to existing features on a regular basis. You can make our job easier by letting us know what you need. Here are a couple of ideas which users requested which may be of interest to you.

HCOMP® TABLE

HCOMP is a Compositional Multiphase Pipeline Model which is owned by Scientific Software, Inc./ Intercomp. HCOMP models fluid systems using a compositional approach. Fluid data may be supplied in tabular form as input to this program. Now DESIGN II can create this table of viscosity, enthalpy, entropy, vapor fraction, and component molar flow versus temperature and pressure using any of the large number of thermodynamic correlations available. This feature is available on PRIME and IBM versions of DESIGN II and it's easy to use. Just ask us how.

LIQUID-LIQUID EXTRACTION

You are probably familiar with the classical countercurrent multiple-contact extraction shown in the diagram below.



This feature will be available to you in a later version of DESIGN II. Let us show you what the test version of our model can do. Using an example from R. E. Treybal's book, *Liquid Extraction*, we get the following results for a system with 50 pounds per hour each of acetone and water and 30 pounds per

hour of 1,1,2-trichloroethane as solvent. The small differences are attributable to 6 stages versus 5.2 stages and adiabatic (enthalpy balance is checked in our model) versus isothermal calculations.

	ChemShare	Treybal
Extract Product (lb/hr)	79.95	80.8
Raffinate	49.98	49.2
Acetone in Extract	46.83	45.1
Raffinate Composition		
$CL_2HC\text{-}CH_2CL$	0.754	0.3
Acetone	3.110	4.92
Water	46.11	43.98
Extract Composition		
$CL_2HC\text{-}CH_2CL$	29.21	29.7
Acetone	46.83	45.1
Water	3.91	6.02
Number of Stages	6	5.2
Temperature variation	Yes	No
K-values	LLE data from I&EC fitted to UNIQUACK	LLE data from I&EC

References: Ind. & Eng. Chem., Vol. 38, p. 817 (1946).
R. E. Treybal, Liquid Extraction, 2nd Ed., p. 234, McGraw-Hill Book Co., Inc. (1963).

Call us if you would like the complete output for this problem.

THERMODYNAMIC UPDATES

SELEXOL® IMPROVEMENTS*

You have probably noticed small changes from previous simulations using the SELEXOL thermodynamic options in version 1.0 of DESIGN II. Several improvements have been supplied to us by the Norton Company, owners of SELEXOL solvent. These modifications are as follows:

1) the heat of absorption of CO_2 in SELEXOL has been improved.

2) the K-value of water has been altered slightly, which should improve pressures and temperatures in the reboiler section of the regenerator.

3) SELEXOL now has a small but finite K-value, which had previously been set to zero. The effect of this change is to model solvent losses.

4) a liquid viscosity correlation for SELEXOL has been added. This new correlation is based on data for CO_2, SELEXOL and water. Since the correlation is new, values in the simulation may differ slightly from those shown in the SELEXOL Design Manual.

In addition to the changes listed above, the list of components which may be used with the SELEXOL thermo options has been expanded. For review, the previous list contained the following:

AMMONIA
ACETYLENE
BENZENE
N-BUTANE
CARBON DIOXIDE
CARBON DISULFIDE
CARBON MONOXIDE
CARBONYL SULFIDE
ETHANE
ETHYLENE
N-HEPTANE
N-HEXANE
HYDROGEN
HYDROGEN CYANIDE
HYDROGEN SULFIDE
ISOBUTANE
ISOPENTANE
METHANE
METHYL MERCAPTAN
NITROGEN
N-PENTANE
PROPANE
THIOPHENE
WATER

The chemicals shown below have been added to the list.

DICHLOROMETHANE
ETHANOL
N-NONANE
N-OCTANE
PERCHLOROETHYLENE
TOLUENE
TRICHLOROETHYLENE
UNDECANE
P-XYLENE

These are the only components for which data has been supplied on absorption in SELEXOL. If you use other components, the program will use the Chao-Seader (STDK) equation to calculate a K-value for that component. If you have any questions, please call Dr. John Adams at ChemShare—(713) 627-8945.

*These changes are also available in DESIGN/2000, version 10.0.

UNIFAC UPDATE

There have been several changes and additions to UNIFAC groups which we have incorporated in ChemTran and DESIGN II. A misprint for the volume parameter (R) for the CCL group has been corrected. Parameters for the OH and C = C groups with most other carbon groups have been revised. In addition, eight completely new groups have been added. The new groups are shown in the table below.

Main group	Sub group	Sample group assignment
"$(C)_3N$"	CH_3N	trimethylamine: 2*CH3,1*CH3N
	CH_2N	triethylamine: 3*CH3,2*H2,1*CH2N
"HCOO"	HCOO	ethyl formate: 1*CH3,1*CH2,1*HCOO
iodide	I	iodoethane: 1*CH3,1*CH2,1*I
bromide	BR	bromomethane: 1*CH3,1*BR
furfural	FURFURAL	furfural: 1*FURFURAL
"pyridine"	C_5H_5N	pyridine: 1*C5H5N
	C_5H_4N	3-methylpyridine: 1*CH3,1*C5H4N
	C_5H_3N	2,3-dimethylpyridine: 2*CH3,1*C5H3N
"DOH"	$(CH_2OH)_2$	1,2-ethanediol: 1*(CH2OH)2
methanethiol	CH_3SH	methanethiol: 1*CH3SH
	CH_2SH	ethanethiol: 1*CH3,1*CH2SH

These modifications are available in ChemTran versions 9.0 or greater and DESIGN II versions 1.0 or greater (also available in DESIGN/2000 versions 9.0 thru 10.0).

MIXDAT - NOW A VLE AND LLE DATABASE

MIXDAT is a new way of retrieving VLE data from the literature. It has been available on ChemShare's computers for about one year. This program offers a means of interactively searching all of the published data for exactly the chemicals, temperature and pressure ranges of interest to you. Up to this time, MIXDAT has consisted of the Dortmund Database which was compiled by Dr. J. Gmehling and Dr. U. Onken at the University of Dortmund in Dortmund, Germany. We have now added a second database to MIXDAT. This is the Lyngby Database for LLE (liquid-liquid equilibrium) data which was compiled by Dr. Aage Fredenslund and his coworkers in Lyngby, Denmark. Together, these two databases contain all data published for VLE and LLE systems from the early 1880's through 1982. These two groups are continuing to collect data and it will be added to MIXDAT on a regular basis.

Combined with ChemTran, this database offers you one of the surest and quickest methods anywhere of developing thermodynamic correlations to accurately simulate chemical systems. The interactive database allows you to quickly select all of the literature data for your chemical mixture for the exact pressure, temperature or concentration range. Perhaps, just as important, it helps you quickly determine if there is no data published for your system. In this case, the UNIFAC option in ChemTran is available to help estimate the non-ideal behavior for your system.

MIXDAT has a menu which guides you through the search process. Most users need little assistance in using this menu since it is self-instructive. There are several categories of information which you can use to locate data. These include

1) number of chemicals in the mixture
2) isobar or isotherm
3) identity of one or more of the chemicals
4) pressure range in mmHg
5) temperature range in degrees C
6) year data was published
7) VLE or LLE
8) type of data reported

Each of these categories can be used singly or in combination. For example, it is possible to find all of the data for mixtures containing cumene which have been published. By adding another category, the data could be limited to all of the LLE data for mixtures with cumene. If you were only interested in data which was published in the last two years, you would add category 6 and specify 1980 and 1982. The results of your search can be printed at your terminal, reviewed on a CRT or stored in a permanent file.

Some interesting data can be obtained from MIXDAT. The LLE database contains about 3000 data sets for a total of 15667 data points. The VLE database contains 9687 data sets for a total of 143002 data points. VLE data has been measured from 1 mmHg to about 150000 mmHg. One of the earliest data sets measured is for water and carbon disulfide. It is LLE data and was reported by G. Chancel and F. Parmentier in the journal Compt. Rendu in 1885.

The results for a search for VLE data for the system water and 1-butanol are shown below. The search was limited to binary data published between 1970 and 1975. If you have further questions or want more detailed documentation, please call Dr. John Adams at (713)627-8945.

```
*******************************************************************************

                    VLE  DATABASE      SEARCH  NO.   1

*******************************************************************************
-------------------------------------------------------------------------------

                         DATA  SET      NO.   1

-------------------------------------------------------------------------------

                        VAPOR-LIQUID EQUILIBRIUM DATA
(1)  WATER                                                          H2O
(2)  1-BUTANOL                                                      C4H10O

TEMPERATURE =       60.00  DEGREES C

AUTHOR    -  SCHREIBER E.,SCHUETTAU E.,RANT D.,SCHUBERTH H.
JOURNAL   -  Z.PHYS.CHEM.(LEIPZIG) 247,23(1971).

PRESS. UNITS: MM HG        CONC. UNITS: MOLE FRACTION

                LIQUID PHASE          VAPOR PHASE

   PRESSURE        CONC(1)               CONC(1)
     62.40          0.0000                0.0000
     91.90          0.0500                0.3540
    115.20          0.1000                0.5100
    148.90          0.2000                0.6540
    168.30          0.3000                0.7230
    179.20          0.4000                0.7600
    185.60          0.5000                0.7810
    187.10          0.5620                0.7860
    187.10          0.6000                0.7860
    187.10          0.7000                0.7860
    187.10          0.8000                0.7860
    187.10          0.9000                0.7860
    187.10          0.9840                0.7860
    149.40          1.0000                1.0000
```

DATA SET NO. 2

VAPOR-LIQUID EQUILIBRIUM DATA

(1) WATER H2O
(2) 1-BUTANOL C4H10O

PRESSURE = 760.00 MM HG

AUTHOR - KATO M.,KONISHI H.,HIRATA M.
JOURNAL - J.CHEM.ENG.DATA 15,435(1971).

TEMP. UNITS: DEGREES C CONC. UNITS: MOLE FRACTION

	LIQUID PHASE	VAPOR PHASE
TEMPERATURE	CONC(1)	CONC(1)
109.30	0.0750	
101.60	0.1890	
97.90	0.2710	
95.00	0.3570	
93.70	0.4340	
92.80	0.5260	
92.40	0.6150	
92.30	0.9570	
93.60	0.9830	
97.30	0.9950	

DATA SET NO. 3

VAPOR-LIQUID EQUILIBRIUM DATA

(1) WATER H2O
(2) 1-BUTANOL C4H10O

PRESSURE = 20.00 MM HG

AUTHOR - FROLOVA E.A.,USTAVSSHIKOV B.F.,PAVLOV S.YU.,
JOURNAL - ZH.FIZ.KHIM. 48,1865(1974).

TEMP. UNITS: DEGREES C CONC. UNITS: MOLE FRACTION

	LIQUID PHASE	VAPOR PHASE
TEMPERATURE	CONC(1)	CONC(1)
41.20	0.0000	0.0000
36.67	0.0500	0.3120
33.52	0.1000	0.5480
28.64	0.2000	0.7980
23.95	0.3000	0.8000
22.05	0.4000	0.8040
20.59	0.5000	0.8080
18.90	0.6000	0.8140
18.90	0.7000	0.8190
18.72	0.8000	0.8200
19.17	0.9000	0.8490
20.64	0.9500	0.9080
20.00	1.0000	1.0000

NEW CORRELATION CAPABILITIES

Several new features have been added to VLE and LLE data reduction in ChemTran offering new capabilities as well as making data entry more convenient. These features are available in version 10.0 of ChemTran. The data reduction capabilities have been extended to handle virtually any form of equilibrium data with liquid and vapor phases. In the past, ChemTran could handle multicomponent mixture data easily. Now it can process multicomponent and multiphase data with equal ease.

VLLE and LLLE Data Correlation

ChemTran can now correlate mixture data for systems with a vapor in equilibrium with two liquid phases, or for mixtures with three liquid phases in equilibrium. The commands for entering these forms of data are extensions of existing commands for VLE and LLE data. For example,

T-P-Y-X-X (units)i, j, k, . . . = data
P-Y-X-X (units) i, j, k, . . . = data
T-Y-X-X (units) i, j, k, . . . = data
T-X-X-X (units) i, j, k, . . . = data

where i, j and k are component ID numbers.

The first command is for VLLE data with both temperature and pressure varying, the second is for isothermal VLLE data and the third is for isobaric VLLE data. The last command is for LLLE data. The conventions for entering component ID numbers, units, temperatures, pressures and composition are the same as for VLE and LLE data (please refer to Section 2 of the ChemTran manual).

The following is a ChemTran input file for VLLE data for the mixture ethanol, benzene and water. The UNIQUAC equation is used for this correlation but RENon could have been specified instead. Portions of the results from ChemTran are also shown.

```
NN999.
*SIMULATNEOUS FIT OF DATA FOR ETHANOL-
BENZENE-WATER
COM = 1012,40,62
UNIQUACK
T-Y-X-X(MMHG,C)1012,40,62 = 760,
      67.0, .109, .643, .020, .963, .048, .001,
      66.0, .160, .601, .046, .933, .077, .002,
      64.9, .241, .548, .232, .664, .225, .021,
      64.9, .248, .543, .281, .555, .277, .048,
      65.0, .255, .533, .339, .330, .331, .133,
      65.0, .258, .530, .339, .330, .331, .133,
FIL NEW = VLLE,DATA,FIT
END
```

```
********* REDUCTION OF PHASE EQUILIBRIUM DATA FOR SYSTEM  1 ********
        COMPONENTS IN SYSTEM  1
-----------------------------------
 NO.    CODE NO.          NAME
----    --------     ----------------
   1       1012       ETHANOL
   2         40       BENZENE
   3         62       WATER

EQUATION OPTION IS UNIQUAC
NUMBER OF ITERATIONS=    37
SUM OF SQUARES OF THE OBJECTIVE FUNCTION=  0.2250191E 00
STANDARD ERROR OF ESTIMATE=  0.6846821E-01
ROOT MEAN SQUARE OF ERRORS=  0.6455244E-01
```

TYXX DATA SET 1 FOR SYSTEM 1 RMS = 0.6455244E-01

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMPOSITION (MOLE FRACTION) COMP	VAPOR	LIQUID(1)	VALUE OF OBJECT FUNCTION
1	152.588	14.6961	1012	0.109000	0.020000	0.06464
1			40	0.643000	0.963000	-0.00247
1			62	0.248000	0.017000	0.09367
2	150.788	14.6961	1012	0.160000	0.046000	0.00651
2			40	0.601000	0.933000	-0.01169
2			62	0.239000	0.021000	0.11496
3	148.808	14.6961	1012	0.241000	0.232000	0.03554
3			40	0.548000	0.664000	-0.00838
3			62	0.211000	0.104000	-0.07988
4	148.808	14.6961	1012	0.248000	0.281000	0.04994
4			40	0.543000	0.555000	-0.00727
4			62	0.209000	0.164000	-0.11280
5	148.988	14.6961	1012	0.255000	0.339000	0.05104
5			40	0.533000	0.330000	-0.03868
5			62	0.212000	0.331000	-0.06629
6	148.988	14.6961	1012	0.258000	0.339000	0.05687
6			40	0.530000	0.330000	-0.04149
6			62	0.212000	0.331000	-0.06629

TYXX DATA SET 1 FOR SYSTEM 1 RMS = 0.6455244E-01

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMPOSITION (MOLE FRACTION) COMP	VAPOR	LIQUID(2)	VALUE OF OBJECT FUNCTION
1	152.588	14.6961	1012	0.109000	0.048000	0.06714
1			40	0.643000	0.001000	0.03358
1			62	0.248000	0.951000	-0.01491
2	150.788	14.6961	1012	0.160000	0.077000	0.08510
2			40	0.601000	0.002000	0.00677
2			62	0.239000	0.921000	0.00176
3	148.808	14.6961	1012	0.241000	0.225000	-0.04420
3			40	0.548000	0.021000	-0.03150
3			62	0.211000	0.754000	0.02061
4	148.808	14.6961	1012	0.248000	0.277000	-0.05101
4			40	0.543000	0.048000	-0.08490
4			62	0.209000	0.675000	0.02503
5	148.988	14.6961	1012	0.255000	0.331000	-0.00487
5			40	0.533000	0.133000	-0.09994
5			62	0.212000	0.536000	0.01077
6	148.988	14.6961	1012	0.258000	0.331000	0.00097
6			40	0.530000	0.133000	-0.10273
6			62	0.212000	0.536000	0.01077

TYXX DATA SET 1 FOR SYSTEM 1 RMS = 0.6455244E-01

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMPOSITION (MOLE FRACTION) COMP	LIQUID(1)	LIQUID(2)	VALUE OF OBJECT FUNCTION
1	152.588	14.6961	1012	0.020000	0.048000	0.00251
1			40	0.963000	0.001000	0.03605
1			62	0.017000	0.951000	-0.10843
2	150.788	14.6961	1012	0.046000	0.077000	0.07863
2			40	0.933000	0.002000	0.01846
2			62	0.021000	0.921000	-0.11322
3	148.808	14.6961	1012	0.232000	0.225000	-0.07961
3			40	0.664000	0.021000	-0.02313
3			62	0.104000	0.754000	0.10032
4	148.808	14.6961	1012	0.281000	0.277000	-0.10070
4			40	0.555000	0.048000	-0.07768
4			62	0.164000	0.675000	0.13744
5	148.988	14.6961	1012	0.339000	0.331000	-0.05590
5			40	0.330000	0.133000	-0.06150
5			62	0.331000	0.536000	0.07701
6	148.988	14.6961	1012	0.339000	0.331000	-0.05590
6			40	0.330000	0.133000	-0.06150
6			62	0.331000	0.536000	0.07701

******* END PHASE EQUILIBRIUM DATA REDUCTION FOR SYSTEM 1 *********

CHEMSHARE CORRELATION CONSTANTS FOR ALL BINARY PAIRS
FROM UNIQUAC EQUATIONS (BTU/LBMOL)

BINARY PAIR	DATA ORGIN	CONSTANT	VALUE	AVE TEMP (F)
ETHANOL(1012) + BENZENE(40)	DATA	A(1012,40)	-643.076	149.83
		A(40,1012)	1778.37	
ETHANOL(1012) + WATER(62)	DATA	A(1012,62)	6183.05	149.83
		A(62,1012)	-843.434	
BENZENE(40) + WATER(62)	DATA	A(40,62)	1875.00	149.83
		A(62,40)	1978.34	

We can then take the results of the ChemTran data fit for the mixture ethanol, benzene and water and use them in DESIGN II to model flashes. A sample input file using the MULPHA (3-phase flash) module and portions of the output are shown below.

```
AB123.
*THREE PHASE FLASHES
MUL PHA1 = PT1,1,-2,-3,-4
MUL PHA2 = PT2,5,-6,-7,-8
MUL PHA3 = PT5,9,-10,-11,-12
MUL PHA4 = PT6,13,-14,-15,-16
GEN
COM = 1012,40,62
FLO1 = 17.7,160.7,121.6
TP(C,MMHG)1 = 67.0,760
FLO5 = 28.3,153.6,118.1
TP(C,MMHG)5 = 66.0,760
FLO9 = 92.5,99.6,107.9
TP(C,MMHG)9 = 65.0,760
FLO13 = 92.8,99.3,107.9
TP(C,MMHG)13 = 65.0,760
UNIQUACK
CHE FIL = VLLE,DATA,FIT
END
```

STREAM SUMMARY

STREAM NUMBER		1	2	3	4
EQUIP CONXION		FEED-PT1	PT1 -PROD	PT1 -PROD	PT1 -PROD
		(0)-(1)	(1)-(0)	(1)-(0)	(1)-(0)
VAPOR FRACTION		0.79380	1.0000	0.00000	0.00000
TEMPERATURE F		152.59	152.59	152.59	152.59
PRESSURE PSIA		14.696	14.696	14.696	14.696
ENTHALPY BTU/HR		-0.62219E 06	0.18760E 06	-0.10932E 07	-0.17215E 07
LB/FT3	T-P		0.13598	50.456	59.596
S.G.(60F)	STP			0.88319	0.96246
GAL/MIN	STP			17.803	4.0724
MMSCF/DAY	STP		0.87731		
MOLECULAR WT		51.860	59.509	75.995	19.571
FLOW RATES	LBMOL/HR				
ETHANOL		17.700	9.9557	2.4474	5.2969
BENZENE		160.70	61.865	98.714	0.12144
WATER		121.60	24.504	2.3335	94.762
TOTAL	LBMOL/HR	300.00	96.325	103.49	100.18
TOTAL	LB/HR	15558.	5732.2	7865.1	1960.7

STREAM SUMMARY (CONTINUED)

STREAM NUMBER		5	6	7	8
EQUIP CONXION		FEED-PT2	PT2 -PROD	PT2 -PROD	PT2 -PROD
		(0)-(2)	(2)-(0)	(2)-(0)	(2)-(0)
VAPOR FRACTION		0.78373	1.0000	0.00000	0.00000
TEMPERATURE F		150.79	150.79	150.79	150.79
PRESSURE PSIA		14.696	14.696	14.696	14.696
ENTHALPY BTU/HR		-0.65927E 06	0.18316E 06	-0.10870E 07	-0.16934E 07
LB/FT3	T-P		0.13545	50.512	58.681
S.G.(60F)	STP			0.88132	0.94091
GAL/MIN	STP			17.396	4.4896
MMSCF/DAY	STP		0.87016		
MOLECULAR WT		51.429	59.101	74.994	20.677
FLOW RATES	LBMOL/HR				
ETHANOL		28.300	14.445	4.7430	9.1123
BENZENE		153.60	58.579	94.748	0.27219
WATER		118.10	22.517	2.7697	92.814
TOTAL	LBMOL/HR	300.00	95.540	102.26	102.20
TOTAL	LB/HR	15429.	5646.6	7669.0	2113.1

STREAM NUMBER		9	10	11	12
EQUIP CONXION		FEED-PT5	PT5 -PROD	PT5 -PROD	PT5 -PROD
		(0)-(3)	(3)-(0)	(3)-(0)	(3)-(0)
VAPOR FRACTION		0.63957	1.0000	0.00000	0.00000
TEMPERATURE F		148.99	148.99	148.99	148.99
PRESSURE PSIA		14.696	14.696	14.696	14.696
ENTHALPY BTU/HR		-0.11136E 07	0.17475E 06	-0.10821E 07	-0.15145E 07
LB/FT3	T-P		0.13070	50.597	55.161
S.G.(60F)	STP			0.84820	0.87076
GAL/MIN	STP			13.635	6.6144
MMSCF/DAY	STP		0.85141		
MOLECULAR WT		46.616	56.891	58.189	26.902
FLOW RATES	LBMOL/HR				
ETHANOL		92.500	27.187	37.448	27.865
BENZENE		99.600	47.784	48.986	2.8302
WATER		107.90	18.510	12.989	76.401
TOTAL	LBMOL/HR	300.00	93.482	99.422	107.10
TOTAL	LB/HR	13985.	5318.2	5785.3	2881.1

STREAM NUMBER		13	14	15	16
EQUIP CONXION		FEED-PT6	PT6 -PROD	PT6 -PROD	PT6 -PROD
		(0)-(4)	(4)-(0)	(4)-(0)	(4)-(0)
VAPOR FRACTION		0.63754	1.0000	0.00000	0.00000
TEMPERATURE F		148.99	148.99	148.99	148.99
PRESSURE PSIA		14.696	14.696	14.696	14.696
ENTHALPY BTU/HR		-0.11209E 07	0.16703E 06	-0.11220E 07	-0.15211E 07
LB/FT3	T-P		0.13070	50.597	55.161
S.G.(60F)	STP			0.84820	0.87077
GAL/MIN	STP			14.137	6.6426
MMSCF/DAY	STP		0.81378		
MOLECULAR WT		46.584	56.891	58.187	26.901
FLOW RATES	LBMOL/HR				
ETHANOL		92.800	25.986	38.831	27.983
BENZENE		99.300	45.672	50.787	2.8410
WATER		107.90	17.692	13.471	76.737
TOTAL	LBMOL/HR	300.00	89.350	103.09	107.56
TOTAL	LB/HR	13975.	5083.2	5998.4	2893.4

SIMULTANEOUS DATA CORRELATION

In addition to permitting VLLE and LLLE data as input, ChemTran will simultaneously regress all forms of data entered for multicomponent mixtures. This is especially important in order to obtain a good representation of both the VLE and LLE behavior in a mixture for three-phase flashes. For the mixture benzene, methanol and water, there is VLLE data as well as VLE and LLE data. This data exists in both ternary and binary form. ChemTran can accept all forms of data and regress it simultaneously. The following input illustrates this capability for the ternary system propanol, butanol and water:

```
NN999.
*SIMULTANEOUS FIT OF VLE AND LLE DATA
COM=1022,1019,62
C-
C- AUTHOR - NEWSHAM, D.M.T., VAHDAT, N.
C- JOURNAL - CHEM. ENG. J., 13, P. 27 (1977)
C-
T-Y-X (MMHG,C)1019,1022,62=739.2,
      90.24, .0605, .0938, .1483, .1477,
      90.22, .0430, .0645, .1492, .1440,
      89.99, .0593, .0683, .1668, .1324,
      89.93, .0544, .0528, .1815, .1225,
      89.72, .0577, .0440, .1899, .1173,
      89.65, .0771, .0700, .1952, .1086,
C-
C- AUTHOR - MCCANTS, J.F., JONES, J.H., HOPSON, W.H.
C- JOURNAL - IND. ENG. CHEM., 45, P. 454 (1953)
C-
T-X-X(MASFRAC,F)1022,1019,62=1.0,
      100.00, .677, .101, .074, .028,
      100.00, .614, .143, .075, .040,
      100,00, .502, .198, .076, .065,
C-
C- USE UNIQUAC EQUATIONS
C-
UNIQUACK
VARY 1022,1019=B12,B21
VARY 1022,62 =B12,B21
VARY 1019,62 =B12,B21
END
```

SIMPLIFIED DATA ENTRY

With the new commands and structure for data entry, several simplifications are possible for your input. For example, when both binary and ternary data are available for the same mixture, they can be entered on separate commands. If we had wanted to add binary VLE data for propanol and water in the input file above, we would simply add a command of the form

```
T-Y-X (units)1019,62 = data
```

ChemTran automatically concatenates all data sets containing data for the same chemicals.

This also permits simple entry of data from different sources which have different units. It is no longer necessary to convert your input to the same set of units. For example, the binary data for propanol and water could be in mmHG and degrees C from one source and PSIA and degrees F from another. The data entries would look like the following:

```
T-Y-X(MMHG,C)1019,62=data
                .
                .
                .
T-Y-X(PSIA,F)62,1019=data
                .
                .
                .
```

Note that the order of component ID numbers can also be different. Another degree of flexibility has been added in the order in which mixture data can be entered. The command T-Y-X indicates that the vapor compositions are entered first followed by the liquid compositions. Now it is possible to also use the command T-X-Y and enter the liquid compositions first followed by the vapor compositions. This allows you to enter the data in the same order as it is tabulated.

You can now enter comment lines in your ChemTran input file. Simply begin each comment line with a C- .

```
C- DATA FROM LAB
C- MEASURED BY J. SMITH ON 2 MAY 79
```

SOURCE CODE FOR SALE

We are now making the source code or object code for ChemTran and DESIGN II programs available for sale. Both programs run on Apollo, IBM, ICL, CDC, DEC, PR1ME and UNIVAC computers. For those companies who are developing their own software, this is a unique opportunity to purchase commercial software.

A brief review of each program's capabilities follows. ChemTran has two major functions:

A. Pure component properties

   1. Data base of 860 pure components

   2. Physical properties generator from a simple structure input

B. Mixture properties

   1. Regress equilibrium data. Data can be VLE and/or LLE, binaries or multicomponent.

   2. Wide choice of thermodynamic options for data regression, including UNIFAC.

   3. Results include graphs and tables of equilibrium data fit.

The output from ChemTran is the printed report plus an optional thermophysical property data file. This file contains properties and coefficients that are used for heat and material balance calculations in a flowsheet simulator. The ChemTran file can be modified to pass this data to programs other than DESIGN II.

DESIGN II, which is described in detail in this newsletter, is the most comprehensive process simulator available. Its broad capabilities cover applications in gas processing, refining, petrochemicals and chemicals.

Questions related to purchase options should be directed to the sales staff at (713)627-8945 or TWX: 910-881-2793.

For better process simulations

Now you can own the world's most powerful mixture-properties generator.

How powerful? How else would you compile binary interaction data for a mixture of 2,3,4-trimethylpentane, 4-hydroxy-4-methyl-2-pentanone, methanol and benzene?

Here's how you could compile the data for this mixture in a matter of hours, instead of days, weeks, or not at all. ChemTran[SM] is the fastest, easiest, and often the only way to obtain pure component and mixture data and then evaluate it for use with Design II[SM] or any other process simulator.

This example shows how you could combine any experimental data you have with ChemTran's large physical properties data base and powerful estimating techniques to characterize this difficult, four-component mixture.

Methanol and benzene properties are easy.

The physical properties of methanol and benzene are contained in ChemTran's pure component data base, which holds properties for more than 850 chemicals. These properties are automatically retrieved as needed for calculations. All you have to do is enter the component ID numbers.

You have properties for 2,3,4-trimethylpentane.

This chemical is in the ChemTran data base, but you can easily enter your own data obtained elsewhere. ChemTran lets you enter properties such as boiling point, critical properties, acentric factor and so on. If your data is incomplete, you can combine what you have with your choice of ChemTran's predictive techniques to formulate complete thermodynamic properties for this chemical.

No physical properties for 4-hydroxy-4-methyl-2-pentanone? No problem.

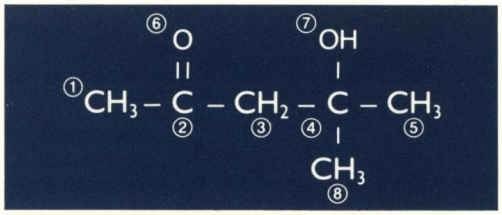
Even when you have no physical properties for a chemical, you aren't at a dead-end. With ChemTran, you can enter the chemical's structure (see box), and ChemTran automatically selects the appropriate group contribution techniques and correlations to estimate the necessary properties, including critical temperature, pressure and volume, solubility parameter and ideal gas heat capacity.

You have binary data only for methanol and benzene? Still no problem.

Experimental vapor-liquid-equilibrium data for the methanol/benzene interaction is readily available, so all you have to do is enter your choice of data. ChemTran is the only program of its kind that can simultaneously regress multicomponent, VLE, LLE, LLLE, VLLE and VLLLE data. The program correlates the data you enter and calculates your choice of Wilson, UNIQUAC or Renon parameters.

Even though no mixture data is available for the other five binary interactions in the mixture, you can still generate parameters with ChemTran's powerful estimation techniques. Using UNIFAC, ChemTran calculates infinite dilution coefficients, which are then transformed into parameters according to the equation option you choose.

Properties predicted from structure



Even if you have only a chemical's structure, the ChemTran program can estimate all necessary physical properties using group contribution techniques and property correlations. All you have to do is enter the structure as shown here. There is no need to enter hydrogens, and you can number the non-hydrogen atoms as you wish:

STRUCTURE 204 = C1–C2, C2 = O6, C2–C3, C3–C4, C4–C5, C4–O7, C4–C8

How much time does all this take?

About two hours. That includes typing in all your data and the necessary commands to control the mixture simulation. The printout includes all of the tables and graphs you need to fully evaluate the data before you use it in your simulation. In addition, the output data is stored on your computer for access by your process simulator.

And now you can own the source.

For the first time, The ChemShare Corporation is offering the ChemTran program for purchase. For more information, write or call ChemShare, and we'll send you a printout of the example described in this ad, complete with input and output, plus additional information on ChemTran.

ChemShare®

The ChemShare Corporation
1900 Lummus Tower • Houston, Texas 77056
Phone: 713/627-8945 • TWX: 910-881-2793 • Hot Line: 713/627-1760

ChemShare Process Systems Ltd.
Brook House Church Street • Wilmslow, Cheshire SK9 1AT England
Phone: 0625-532113 • Telex: 666905