DESIGN II℠ AND CHEMTRAN® NEW FEATURES UPDATE

MARCH 1991

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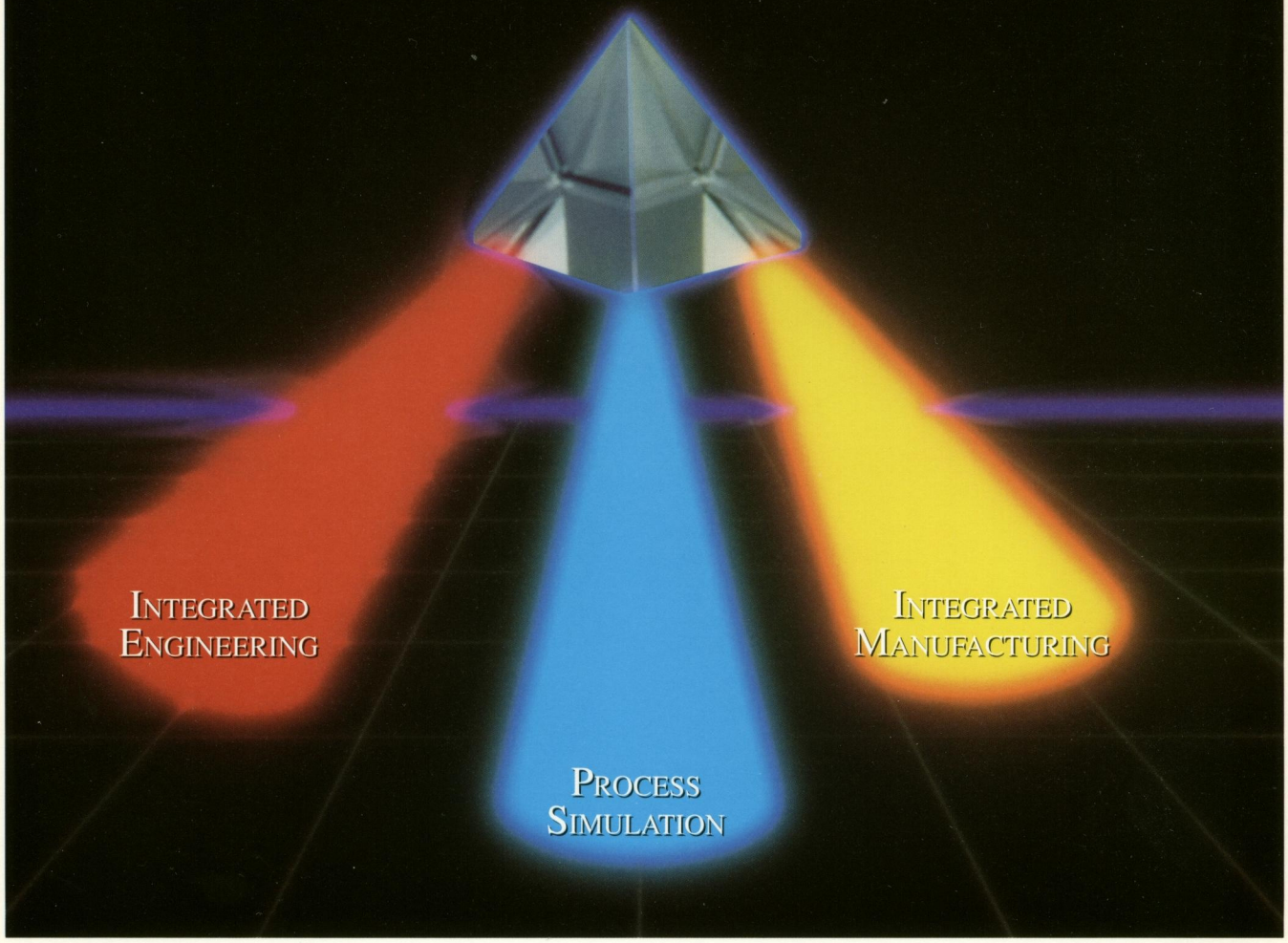

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20 YEARS OF EXCELLENCE BY DESIGN

ChemShare's Process Simulation Division is proud to bring you our latest DESIGN II Version 6.0 and ChemTran Version 16.0. We believe these new capabilities will extend your application range of ChemShare's simulation products. Our goal is to provide you with new technology and increased flexibility to compliment your engineering talents.

This ChemShare New Features Update includes all the technical documentation required to apply the new features. If you need any further explanations, please contact the ChemShare Technical Service department at 713-267-5678 (U.S.A.) or your local ChemShare office.

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New Features and Enhancements Summary

Pipeline Heat Transfer to the Surroundings

You now have added flexibility in calculating heat transfer to the surroundings. DESIGN II estimates the overall heat transfer coefficient, U, if it is not specified. Insulation thickness of each layer is to be specified, and 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.

DESIGN II Keyword Commands

Pipe Material

To specify pipe material:

PIPe **MAT**erial = one of the following keyword choices

Material	Keyword
• Carbon steel (default)	**CAR**bon
• Admiralty brass	**ADM**iralty brass
• Stainless steel	**STA**inless steel
• Aluminum	**ALU**minum
• Monel	**MON**el
• Red brass	**RED** brass
• Copper	**COP**per
• Copper nickel 90/10	**COP**per **90**/10
• Copper nickel 70/30	**COP**per **70**/10
• Nickel	**NIC**kel

Pipe Thickness

Two commands are available to specify the pipe thickness. These are:

PIPe **WAL**l Thickness = **STD, XS,** or **XXS** (STD is default)

or

PIPe **THI**ckness (L units) =

These commands must be used in combination with the NOMinal DIAmeter or the INSide DIAmeter commands.

Pipe Insulation

The keywords to define the insulation are as follows:

INSulation **THI**ckness (L units) n = insulation thickness of the n^{th} layer.
INSulation **CON**ductivity (k units) n = thermal conductivity of the n^{th} 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. Please see *DESIGN II User's Guide* Page 5.13.1 and Example Problem 1.

Thermal Conductivity of Surroundings

To specify the thermal conductivity of the surroundings, enter the following commands:

SURrounding **SOI**l **CON**ductivity (k units) = thermal conductivity of the soil
SURrounding **WAT**er **CON**ductivity (k units) = thermal conductivity of the water
SURrounding **AIR CON**ductivity (k units) = thermal conductivity of the air

Only the following units are allowed for thermal conductivity input units (k units):

British (default)	SI	Metric
BTU/HR/FT/F	KJ/S/M/K	KCAL/HR/M/C

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 =	**SAN**d **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)
SURrounding **WAT**er	(default	k= 0.3517)
SURrounding **AIR**	(default	k= 0.015)

VELocity of **SUR**roundings (L units/t units) = (required if submerged in water or exposed to air. Default = 0)
PIPe **DEP**th (L units) = depths at which pipe is buried under soil or water. Values must be given for each line segment.

Temperature of Surroundings

The temperature of the surroundings is specified with the TEMperature SURroundings = command. See the *DESIGN II User's Guide* page 5.13.5.

Example

The following example demonstrates the new pipeline heat transfer to surroundings options. A line 16 inches in diameter and 10 miles long is shown. This line slopes upwards for an elevation change of 10 feet over the first mile, 10 feet over the second mile and so on for a total elevation change of 117 feet over 10 miles. The insulated line is submerged in water of 60 F.

```
. . .
LINe 8 = LINE,11,-12,
    NOMinal DIAmeter (IN) = 16,
    LENgth (MILES) = 10*1,
    ELEvation (FT) = 3*10, 5, 2, 20, 30, 3*10,

C-  The surrounding water is at a temperature of 60 degrees F.
    TEMperature SURroundings = 10*60,
    PIPe MATerial = CARBON STEEL,

C-  The flow of the water is 10 ft/second.
    VELocity SURroundings (FT/SEC)=10*10,
    SURrounding WATer CONductivity (BTU/FT/HR/F)=10*0.11,

C-  The line is protected by two layers of insulation.
C-  Each layer is described by thickness and conductivity.
    INSulation THIckness   (IN) 1      = 10*2,
    INSulation CONductivity (BTU/FT/HR/F) 1= 10*0.05,
    INSulation THIckness   (FT) 2      = 10*0.5,
    INSulation CONductivity (KCAL/M/HR/C) 2= 10*0.027,
. . .
```

New Methods for Pipeline Calculations

Frictional Pressure Drop, Liquid Holdup and Flow Regime Correlations

Four additional frictional pressure drop correlations and three additional holdup correlations are available in DESIGN II.

Pressure drop	Holdup	Flow Regime
* Mukherjee-Brill	* Mukherjee-Brill	Baker
* Hagedorn-Brown	* Duns-Ros	Beggs-Brill
* Duns-Ros	* Lockhart-Martinelli	* Mukherjee-Brill
* Oliemans	Hughmark	* Duns-Ros
Darcy-Weisbach	Dukler	
Lockhart-Martinelli	Eaton	
Orkiszewski	Hughmark and Pressburg	
AGA	Beggs and Brill	
Weymouth		
Panhandle A		
Modified Panhandle		
Dukler		
Beggs and Brill		

* new

Applications

Mukherjee-Brill:	Two-phase flow in horizontal, inclined, or vertical pipes.
Duns-Ros:	Two-phase flow in vertical pipes.
Oliemans:	Two-phase flow in horizontal pipes.
Hagedorn-Brown:	Two-phase flow in vertical pipes.
Lockhart-Martinelli:	Two-phase flow in horizontal pipes.

Refer to the DESIGN II User's Guide Chapter 5.13 for information on existing correlations.

Four Flow Regime methods are now available in DESIGN II: Baker, Beggs-Brill, Mukherjee-Brill, and Duns-Ros. 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 flow regime method is designed for vertical flow and is used when Duns-Ros frictional pressure drop is chosen. The Orkiszewski pressure drop method uses the Duns-Ros flow regime map. Plots are produced for all of these methods. The Baker flow regime correlation is automatically plotted by DESIGN II when any two-phase frictional pressure drop techniques is specified with the exception of Beggs and Brill. Beggs and Brill calculates the flow regime and presents this information in tabular form, not as a plot.

Pressure Drop Due to Fluid Acceleration

The LINe module now includes a method by Duns-Ros to calculate pressure drop due to acceleration. This can be used with all of the existing correlations to compute the total pressure drop. If the user does not specify pressure drop calculation due to fluid acceleration, this will default to zero.

The largest acceleration effect will occur where there is a significant change in velocity such as with phase changes and large overall pressure drops.

DESIGN II Keyword Commands

To calculate pressure drop due to acceleration, give the following GENeral section commands:

METhod **ACC**eleration

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.

Alternate Method Option

The LINe module now allows the specification of two friction pressure drop and friction factor methods. For example, the 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 the user's first choice.

DESIGN II Keyword commands

METhod **FRI**ctional pressure drop	= first choice
METhod **FRI**ctional pressure drop **ALT**ernate	= second choice
METhod **FAC**tor	= first choice
METhod **FAC**tor **ALT**ernate	= second choice

A list of frictional pressure drop and friction factor calculation methods appears on page 4 of this document.

New Pipeline Downstream Pressure Specification

The LINe module now 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. 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 of this improvement include direct calculation of 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. Now you can specify the downstream pressure directly.

DESIGN II Keyword commands

PREssure OUT (P units) =

Example:

```
LINe 10 = P101,2,-3,
     PRE OUT (PSIG) = 350
F-   POST
F-   UPPRE = GET(LINE(10),CALculated UPStream PREssure)
F-    PRINT UPPRE
```

For information on retrieving and printing calculated values such as upstream pressure, see page 12 on Inline FORTRAN.

New Oil/Water Emulsion Viscosity Characterization

DESIGN II now allows user specified oil/water emulsion viscosity characterization. Previously, DESIGN II allowed oil/water emulsion viscosity characterization using the Beggs-Brill method where the emulsion is defined as tight, medium, or loose. Now, emulsion viscosity data at different temperatures can be entered in the GENeral section. The user 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.

DESIGN II Keyword commands

The following is a GENeral section command. This command can be repeated to define different temperatures and different sets.

EMUlsion **SET** (T units) n = T, x_1, r_1, x_2, r_2, ...

where n is the set number, T is the temperature at which data is provided, x_n are the water weight fractions and r_n are the corresponding viscosity **ratios** of emulsion to water.

To specify the emulsion used in the LINe module, you have the following choices:

Existing Options
EMUlsion = **LOO**se
EMUlsion = **MED**ium
EMUlsion = **TIG**ht

New Option
EMUlsion = **SET** n where n is the set number

Example:

```
LINE 1 = P101,1,-2,
. . .
    EMUlsion = SET 1

LINE 2 = P102,20,-30,
. . .
    EMUlsion = SET 2

GENeral
    EMUlsion SET (C) 1 = 100.0, 0.1, 1.1, 0.2, 1.2,.....

    EMUlsion SET (C) 1 = 120.0, 0.05, 1.11, 0.2, 1.5, ....

    EMUlsion SET (C) 2 = 70.0, 0.1, 1.2, 0.23, 1.6, .....
END
```

This example shows two emulsion sets, 1 and 2. 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 viscosty.

Line Module References

(1) Mukherjee, H. K., " An Experimental Study of Inclined Two Phase Flow", U. of Tulsa, Ph.D dissertation (1984).

(2) Hagedorn, A. R., "Experimental Study of Pressure Gradients Occurring During Vertical Two Phase Flow in Small-Diameter Conduits", The U. of Texas, Ph.D dissertation (1964).

(3) Brill, J. P., and Beggs, H. D., *Two-Phase Flow in Pipes*, Third printing, Van Nostrand Reinhold Company, (1984).

(4) Govier and Aziz, *The Flow of Complex Mixtures in Pipes*, Van Nostrand Reinhold Company, New York, New York(1972).

(5) Lockhart, R. W. and Martinelli, R. C., "Proposed Correlation of Data for Isothermal Two-Phase, Two-Component Flow in Pipes", Chem. Eng. Progress, vol 45, p 39 (1949).

(6) Neher, J. H., "The Temperature Rise of Buried Cable and Pipes", Trans. A.I.E.E, 68(1), 9(1949).

(7) Hein, M. A., "Incorporating Rigorous Heat Balance Prevents Overdesign of Gas Pipes", Oil & Gas Journal, Sep 17, p 96(1984).

(8) Engineering Data Book, Chapter 10, 9th Ed., Gas Processors Suppliers Association, Tulsa, OK, (1972).

American Gas Association (AGA) Density Method

The AGA density correlation is a natural gas density prediction method developed by the American Gas Association. The primary applications for the method are in the prediction of density of natural gas, metering of natural gas and in the estimation of gas reservoir reserves.

DESIGN II GENeral Section Keyword Commands

To specify the AGA density method, place the following command in the GENeral section:

AGAD

Applicability

This method is generally applicable for compositions within the following range:

Component	Mole Percent
Methane	50 - 100 %
N_2	0 - 50
CO_2	0 - 50
Ethane	0 - 20
Propane	0 - 5
Butane	0 - 3
Pentane	0 - 2
Hexane and heavier	0 - 1
Water vapor, H_2S, H_2, CO, O_2, He and Argon	0 - 1

Tests performed indicate that the method predicts densities for both liquid and vapor accurately even beyond stated composition ranges. While this method can be used at pressures above 20,000 psia and temperatures above 400 degrees F, results should be viewed with caution and reduced accuracy should be expected.

References

Compressibility and Supercompressibility for Natural Gas and Other Hydrocarbon Gases, Transmission Measurement Committee Report No. 8, AGA Catalog No. XQ1285, December 1985, pp 1 - 12

New Orifice Discharge Coefficient Method

DESIGN II now offers the API method for calculating the coefficient of discharge for the flow meter module (FMTR). It is for use with square-edged, flange-tapped orifice meters only. The coefficient of discharge equation was developed by Reader-Harris/ Gallagher and is applicable to both single and two-phase flow.

DESIGN II Keyword Commands

This equation is now available to DESIGN II users in the Flow meter (FMTR) module by using the following keywords:

METhod = API

Reference

Manual of Petroleum Measurement Standards, Chapter 14, Section 3, part 1.7.2, American Petroleum Institute, Committee on Petroleum Measurements, Washington, D.C., August, (1990).

New Oil-Gas-Water Equation of State, Soave-Kabadi-Danner

ChemShare has implemented the Soave-Kabadi-Danner K-value, enthalpy and density methods based upon a modified Soave-Redlich-Kwong equation of state. This equation of state is particularly suitable for two and three phase equilibrium calculations for water-hydrocarbon systems.

DESIGN II Keyword Commands

To specify the Soave-Kabadi-Danner equation of state, the following keywords should be entered in the GENeral section:

SKDK, SKDH, SKDD

Limitations

This method applies only to hydrocarbon-water systems. If water is not present in the system, then the SKD method defaults to APISOAVE.

For accurate predictions of three phase separation, the MULtiple PHAse flash module *must* be used. For all other units, the immiscible water flash method described on page 7.2.15 of the *DESIGN II User's Guide* is used.

The correlation was developed for hydrocarbons up to C_{10} and should give reasonable results at temperatures up to 550 F. Caution should be used in applying this method to hydrocarbons heavier than C_{10} or close to the three phase critical point. SKD gives better results and is applicable over a wider range of temperatures than the UNIFAC correlation.

A group contribution method is used to determine interaction parameters for the following classes of hydrocarbons. If a hydrocarbon in your system is not in one of these classes, use of the SKD method is not recommended.

Homologous Series

Alkanes
Alkenes
Dialkenes
Acetylenes
Naphthenes
Cycloalkenes
Aromatics

For non-hydrocarbons, interaction parameters default to zero.

References

(1) American Petroleum Institute Technical Data Book, Chapter 9, pp 9-111 to 9-115, Port City Press, Washington, D.C. (1982). Third Revision.

(2) Soave, Giorgio, "Equilibrium Constants from a Modified Redlich-Kwong Equation of State", Chem. Eng. Sci., Vol. 27 No. 6, pp. 1197-1203, (1972).

(3) Kabadi,V., Danner, R., "A Modified Soave-Redlich-Kwong Equation of State for Water-Hydrocarbon Phase Equilibria",Ind. Eng. Chem. Proc. Des. Dev., Vol 24, No. 3, pp 537-561 (1985).

Improved Yen-Woods (STD) Density Method

The Yen-Woods correlation for liquid densities is formed from two contributions. The first contribution gives the density of the liquid at its saturation pressure. The second contribution corrects for deviation from saturated conditions. This correction for deviation from saturation has been improved for version 6.0. An additional benefit of the new density correction is that constant volume heat capacity calculations are improved.

Furthermore, DESIGN II now offers a choice of mixing rules for calculating mixture critical properties for the Yen-Woods density

method (STDD). The mixing rule options are Kay and Redlich Kwong. The RK method estimates the critical parameters by finding the values of T_c and V_c that satisfy the critical point conditions for the Redlich Kwong equation of state. For all systems, the RK option will give a better estimate of critical properties than the KAY option. However, KAY will generally yield valid results when the ratio of the largest P_c to the smallest P_c is less than 2.0 **and** the ratio of the largest T_c to the smallest T_c is less than 2.0. Kay is the method which has been used in previous versions of DESIGN II.

Note: Since STDH uses the STDD calculations while determining liquid enthalpies, these modification will also affect STDH calculations.

DESIGN II Keyword Commands

The following command will specify the mixing rule used to determine mixture critical parameters.

YEN WOOds MIX = **KAY** (default)
RK

UNIFACK Applications Extended

Previously, UNIFACK could not be used for user-defined components. In Version 6.0, UNIFACK can be used in DESIGN II for a component for which the structure is defined in ChemTran. A user-defined component can be described by specifying the structure or it can be described by specifying physical properties. Only those components defined by structure can be used with UNIFACK.

Multiple-Phase Flash Extended for Use with Cubic Equations of State

The MULtiple PHAse flash module is used to rigorously separate multiple phase streams. Previously, this module could be used only with activity coefficient K-value options such as RENon, UNIQUAC and UNIFAC. Now, you also have the option of using cubic equations of state such as PENg-Robinson K, SOAVEK, APISOAVEK, MODified PENg-Robinson K, or Soave-Kabadi-Danner (SKDK, released in version 6.0) with the MULtiple PHAse flash module.

ChemTran Enhancement

ChemTran has been extended to allow VLE and VLLE data regressions to all equations of state. To obtain more accurate three phase flash calculations, equilibrium data may be regressed to the desired thermodynamic method with ChemTran.

Example:

```
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
```

Inline Fortran Extensions and Enhancements

DESIGN II offers the ability to directly interface with the flowsheet model through the use of FORTRAN. This feature is called Inline FORTRAN and allows you to access flowsheet parameters and set unit operation specifications by placing FORTRAN commands directly in the input file. The compiling and linking of this code is completely transparent. See *DESIGN II User's Guide* section 9.0 for complete instructions on how to use Inline FORTRAN and refer to 1990 New Features Update for complete list of other parameters available.

A list of new equipment parameters which can be accessed by the GET and SET commands is shown below. The dimensional units shown are the DESIGN II internal units in which the item will be stored.

	Module	**Parameter Description**	**Units**
	STREAM		
	UOPK	UOP K factor	——
	LINE		
	CAL U n	Calculated U factor	BTU/HR/FT2/F
	CAL UPS PRE	Calculated Upstream Pressure	PSIA
Δ	PRE OUT	Pressure Outlet	PSIA
Δ	CON m, SEG n *	Ins. Layer Conductivity per Segment	BTU/HR/FT/F
Δ	INS m, SEG n *	Ins. Layer Thickness per Segment	FT
Δ	VEL SUR n	Velocity of Surrounding	FT/HR
Δ	PIP DEP n	Pipe Depth	FT
Δ	PIP THI n	Pipe Thickness	FT
	SUR WAT CON n	Surrounding Conductivity of Water	BTU/HR/FT/F
	SUR AIR CON n	Surrounding Conductivity of Air	BTU/HR/FT/F
	SUR SOI CON n	Surrounding Conductivity of Soil	BTU/HR/FT/F

HEAt EXChanger

	CAL ARE	Calculated Area	FT2
Δ	EST ARE	Estimated Area	FT2
Δ	NUM FEE 1	Number Shell Side Feeds	——
Δ	NUM FEE 2	Number Tube Side Feeds	——
Δ	PRO 1	Shell Side Phase Separation	——
Δ	PRO 2	Tube Side Phase Separation	——

POLytropic compressor

	CAL POL EFF	Calculated Polytropic Efficiency	——

REFIne

Δ	HEA PUM (i)	Specified heat removed by pumparound(i)	BTU/HR
	CAL HEA PUM (i)	Calculated heat removed for pumparound(i)	BTU/HR
Δ	PRO SPE (i)	Product Specification	——

'm' refers to layer number, 'n' refers to the segment number.

*These FORTRAN keywords require the following format:

variable = GET(LINE(no.), INSulation (mth layer), SEGment (nth segment))

Δ available to SET command as well as GET.

Inline FORTRAN for REFine Tower Compositions

The following Inline FORTRAN commands may be used to retrieve the liquid and vapor compositions on each tray of the REFINE column. These commands must appear in the REFine module to which they pertain.

CALL REF LIQ (X, ITRAY, IFLAG)
CALL REF VAP (Y, ITRAY, IFLAG)

ITRAY = tray for which the liquid/vapor composition is desired. Trays are numbered from top to bottom with the condenser as tray 0.

X/Y = composition of the liquid/vapor. X and Y must be dimensioned equal to the number of components in the component list.

IFLAG = 1 mole fractions
2 mass fractions

Output Control and Suppression

A new command is available to minimize the output from a DESIGN II run. To specify the reduced output format, the following command should be entered in the GENeral section:

PRInt **SWI**tch = 3

This command can be used to reduce the information printed for iterations of a recycle loop.

New Product - DESIGN II/Batch*

ChemShare has significantly increased its range of application with the introduction of a new batch distillation product - DESIGN II/Batch. This is a robust and powerful batch distillation model that is integrated into the DESIGN II flowsheet simulation software. Using DESIGN II/Batch, you will be able to take advantage of DESIGN II's chemical component library, physical properties and thermodynamic correlations and all of DESIGN II's advanced flowsheet technology.

DESIGN II/Batch provides unequaled flexibility and power with the following features:

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

*ChemShare's batch distillation module may not be included in your new program release. It is available as a separate product option and has its own User's Guide. While the batch distillation module uses all of the components, thermodynamic methods and physical properties available to DESIGN II, Batch is an optionally purchased product. Please contact your ChemShare Sales Representative for further information on DESIGN II/Batch.