ChemShare

Newsletter No. 203

Month of Dec. 1982



# VERSION 9.0

# INDEX

CHEMTRAN



Computer Services

## Best Wishes For The New Year

We would like to wish all our readers best wishes for 1983. Most of our readers have had to deal with the bad economic downturn in 1982 and are probably glad it's behind us. The signs for 1983 are already looking better, so let's hope for a stronger economy next year.

## Major Comparisons

Recently we have been involved in evaluations with some major oil companies who were interested in long term access to process simulation software. As far as we know, we were compared with SIMSCI, ASPEN and CONCEPT, and in each case we came out ahead. We normally never publish anything in our newsletter related to these comparisons, but these were so extensive and by such large firms, it is important for our readers to be kept abreast of ChemShare's performance. The companies who did recent evaluations were:

The Abu Dhabi National Oil Company
The British National Oil Company
The Malaysian National Oil Company
SASOL - South African major oil from coal producer

## ICI and ChemShare Work On Integrated Data Base

At the recent AIChE meeting in Los Angeles, John Liles of ICI announced that ICI and ChemShare will be working together to develop and market an integrated data base system which will link to ChemShare's process simulation software. This integrated system has the ability to link to other process engineering related programs such as HTRI and FRI, as well as provide graphics capabilities. The system is presently being developed at ICI's facility in England. Development and test marketing will be done during 1983, and we hope to be able to offer this product to you sometime in late 1983.

## Easier Identification of your Program Versions

In our continued effort to supply you with the latest program features, we are simplifying the way we identify different versions of the programs. In the future, instead of referring to program version "08JUN82 or later" we will refer to a simple version number such as 9.0.

New program features announced in newsletters will specify corresponding program versions in which they are available. The simpler numbering system avoids any confusion over version dates.

The next version released will be 9.0. The full release after that will be 10.0. However, if any additions are made to the 9.0 version before the release of 10.0, the resulting versions will be identified as 9.1, 9.2 etc. The version numbered 9.2 will automatically contain all features included in versions 9.0 and 9.1.

## Summary of Developments in 1982

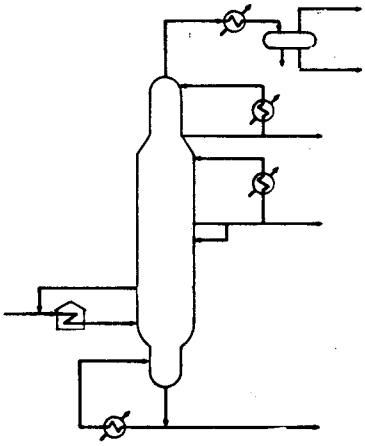
During 1982, we have developed many new features and capabilities. We present these for your review. One of the major differences between our service and our competitors' is the ability to keep adding new technical features that are important to the users. If you compare our December 1981 and December 1982 newsletters with our competitors', you will see that our competition is trying to catch up to us by coming out with capabilities already available in ChemShare. If you don't have any of the newsletters for the past year, please call us for copies.

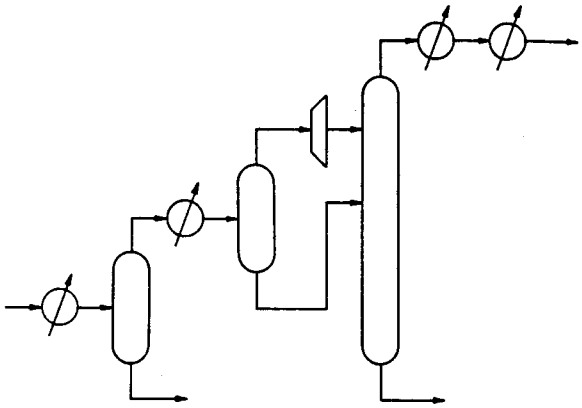
| Feature | Newsletter | Program | Version |
|---|---|---|---|
| Simplified End Points | Dec. 82 | REFINE | 9.0 |
| Feed Phase to Distillation | Dec. 82 | DESIGN | 9.0 |
| FORTRAN-In-Line Code | Feb. 82 | DESIGN | |
| GLITSCH Tray Sizing | Dec. 82 | DESIGN | 9.1 |
| Heating/Cooling Curves | Dec. 82 | DESIGN | 9.0 |
| Line Sizing | May 82 | DESIGN | 9.0 |
| LLE Data Base | Dec. 82 | MIXDAT | |
| Metric and SI Units | Dec. 82 | DESIGN | 9.0 |
| Molecular Weights | May 82 | REFINE | 08 MAR 82 |
| Multiple Flash Unit | Dec. 82 | DESIGN | 9.0 |
| Non-molar Product Specifications | May 82 | DESIGN | 08 MAR 82 |
| Output Tables | Dec. 82 | CHEMTRAN | 9.0 |
| Output Units | Feb. 82 | CHEMTRAN | 01 MAR 82 |
| PENG-Robinson Interactions | Dec. 82 | DESIGN | 9.0 |
| Phase Map for detailed phase envelopes | Dec. 82 | DESIGN | 9.0 |
| Quench Units | Dec. 82 | REFINE | 9.0 |
| Reid Vapor Pressure | May 82 | DESIGN | 08 MAR 82 |
| Remarketing Prime Computers | May 82 | | |
| Reverse Material Balance | Feb. 82 | DESIGN | |
| Selexol Solvent | Feb. 82 | DESIGN | 20 JAN 82 |
| Separator Sizing | Dec. 82 | DESIGN | 9.0 |
| Simplified Feeds | Dec. 82 | DESIGN | 9.0 |
| Sour Water-caustics/acids | May 82 | DESIGN | 08 MAR 82 |
| Transmission Lines | Dec. 82 | DESIGN | 9.0 |
| Viscosity Specifications | May 82 | REFINE | 08 MAR 82 |
| VLE Data Base | Dec. 82 | MIXDAT | |
| Water Decant | Dec. 82 | DESIGN | 9.0 |
| Water Entrainment | Dec. 82 | DESIGN | 9.0 |

## Cost Comparison

ChemShare has continued to hold the line on prices, while our competition has continued to raise their prices. If you use a competitor's software you are probably being overcharged compared to ChemShare's prices. Also most of our competitors bill through computer service bureaus, not directly as we do. The service bureaus add 5 to 15% more to each run for handling money. Therefore, when the competition raises its prices 10% the total increase to you is greater. For example, SIMSCI charges $1.35 per PCU, (not $1.00 as some people think), and then UCS adds 5% and CDC adds 15% for handling charges on every run. Service bureaus also have monthly minimum charges for which you will be billed even if there is no usage. Where ChemShare handles the billing there is no monthly minumum.

Below, we present typical problems useful for comparing costs. You will notice a savings of 35 to 50% using ChemShare over SIMSCI. If any of our readers are using SIMSCI, let us review your typical applications and see if we can help reduce your costs.





CHEMSHARE at $1.40/CCU

60 CCU's = $84.00

SIMSCI at $1.35/PCU

108.09 PCU's

| UCS (+5%) | CDC (+15%) |
|---|---|
| $153.49 | $167.54 |

CHEMSHARE at $1.40/CCU

62 CCU's = $86.80

SIMSCI at $1.35/PCU

92.41 PCU's

| UCS (+5%) | CDC (+15%) |
|---|---|
| $131.22 | $143.23 |

## Now a VLE and a LLE Data Base

ChemShare announced in "Chemical Engineering Progress" (October, 1982) that we have entered into an agreement to exclusively market (except in Europe) the Dortmund VLE Data Base. This data base contains virtually all of the world's published and unpublished VLE data. We have now entered into a similar agreement with Fredenslund and his co-workers in Denmark to market their LLE data. These two important collections of data will be placed in one data base on our computer system.

Work is in progress on the data base which will allow you to have all this data literally at your fingertips. An interactive system is available that lets you search the entire data base at your terminal. Instead of poring over many sources and looking page by page for data you now merely type a command and let the computer do the work for you. With this data base you will be able to get answers to a number of questions instantly.

For example:

1. What VLE data is available for ethanol and benzene?

2. What data is available for these components for a specific temperature range and pressure range?

3. What data has been published for these systems since 1975?

This is just a sample of the variety of queries which can be made to the data base. In addition, ChemTran is available for correlating any data you find from the data search. Thus, there is no guess work about how well correlations work for your system. You can custom design the correlation for yourself and obtain a detailed error report and analysis of the correlation.

Furthermore, these data bases are not static. The Dortmund group and the Fredenslund group are continuing to collect and evaluate more data. This will be provided to ChemShare on a periodic basis and we will keep the data base updated.

The Data Bank now runs on our Prime computers, and is available on a pay-as-used basis, lease or sale. Conversions to IBM, CDC, or UNIVAC computers can be arranged. If you would like further information or technical details, call Dr. John Adams at (713)627-8945.

A sample output of 2 sets of data plus references that you get from this service is shown below.

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VLE DATABASE SEARCH NO. 1

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DATA SET NO. 1

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(1) FORMALDEHYDE CH2O
(2) WATER H2O

TEMPERATURE = 40.00 DEGREE C

AUTHOR - BRANDANI V.,DI GIACOMO G.,FOSCOLO P.U.,
JOURNAL - IND.ENG.CHEM.,PROCESS DES.DEV. 19,179(1980).

| P MM HG | X1 | Y1 |
|---|---|---|
| 55.30 | 0.000000 | 0.000000 |
| 52.90 | 0.029500 | 0.000000 |
| 53.90 | 0.036400 | 0.000000 |
| 53.10 | 0.062700 | 0.000000 |
| 52.50 | 0.067200 | 0.000000 |
| 53.10 | 0.068800 | 0.000000 |
| 51.80 | 0.110300 | 0.000000 |
| 51.00 | 0.156600 | 0.000000 |
| 49.10 | 0.208800 | 0.000000 |
| 47.40 | 0.230200 | 0.000000 |
| 46.10 | 0.279500 | 0.000000 |

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DATA SET NO. 2

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(1) FORMALDEHYDE CH2O
(2) WATER H2O

TEMPERATURE = 50.00 DEGREE C

AUTHOR - BRANDANI V.,DI GIACOMO G.,FOSCOLO P

JOURNAL - IND.ENG.CHEM.,PROCESS DES.DEV. 19,179(1980).

| P MM HG | X1 | Y1 |
|---|---|---|
| 92.50 | 0.000000 | 0.000000 |
| 91.80 | 0.029500 | 0.000000 |
| 90.80 | 0.036400 | 0.000000 |
| 90.80 | 0.036400 | 0.000000 |
| 90.10 | 0.062700 | 0.000000 |
| 90.30 | 0.067200 | 0.000000 |
| 90.70 | 0.068800 | 0.000000 |
| 88.60 | 0.110300 | 0.000000 |
| 86.80 | 0.156600 | 0.000000 |
| 84.40 | 0.208800 | 0.000000 |
| 83.30 | 0.230200 | 0.000000 |
| 80.50 | 0.279500 | 0.000000 |

## Amines Enhancements

Our continuing effort to extend the amine correlations to higher loadings has been very successful. We have tested problems with loadings as high as 2.0 moles of acid gas per mole of amine, and there seems to be no practical upper limit to the loadings that can be handled.

Also, additional work with our rigorous distillation techniques has eliminated the need to enter special convergence commands for amine contactors on version 9.0 or later. For contactors (i.e. absorbers) COMCON=30,3 is no longer required. These new capabilities are available now on our PRIME computer and will be available on other systems during the coming months. If you have been unable in the past to model your amine plant because of the limitations of earlier versions, please give us a call! We'd like to show you what our latest version can do.

## Enhanced Oil Recovery With $CO_2$

Numerous studies are in the works for $CO_2$ flooding of oil fields by many operating companies. ChemShare offers some unique thermodynamic capabilities for these studies which may not be apparent to the casual user of our services. We offer:

1. APISOAVE
2. DORTMUND VLE DATA BANK

The APISOAVE correlation contains VLE data covering a wide range of conditions where high concentrations of $CO_2$ are found. This correlation has data for $CO_2$ concentrations as high as 80% and has been installed in DESIGN/2000 for over a year. All you need to do to run a phase envelope or flash to check the correlation for your mixture is add APISOAVEK in the GENeral section of DESIGN/2000.

The DORTMUND VLE Data Bank is another source of equilibrium data which may contain data for mixtures that can be closer to the mixture you may be studying. For those interactions where there is data, this data can be fit to the APISOAVE equation. For the remainder of the interactions where there is no data, the APISOAVE equation will calculate estimates of interactions based on the acentric factors and solubility parameters for each binary.

With either approach, any customer can easily review these systems and look at alternatives with extremely good results. These options are only available via ChemShare.

## Modeling Ryan/Holmes Processes

Recently many people have expressed an interest in using ChemShare programs to model the Ryan/Holmes processes. This technique for separating acid gases from hydrocarbons uses cryogenic distillation with the addition of butane or heavier hydrocarbons. The additive prevents $CO_2$ freeze-up and $CO_2$ -ethane azeotrope formation. These processes have become increasingly important as we see more $CO_2$ flooding for enhanced oil recovery and development of high $CO_2$ gas fields.

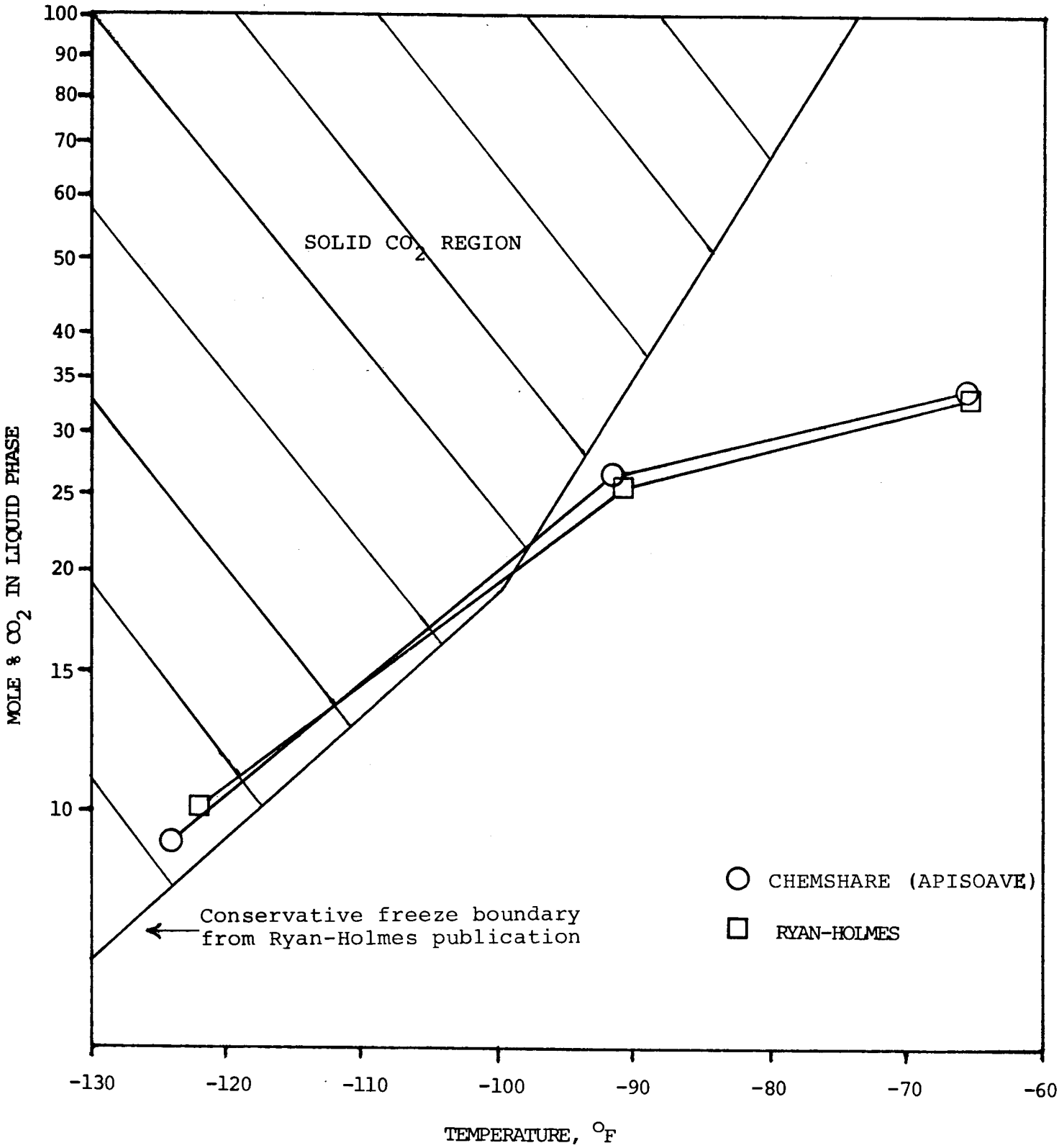
We recently conducted extensive testing of ChemShare's APISOAVE and $CO_2$ FREEZE options for this application. We compared our results to those given in the paper presented by A. S. Holmes, et. al. at the 61st Annual GPA Convention held in Dallas on March 15-17, 1982. In all of the cases tested we found our results were consistent with the Ryan/Holmes results. We also curve fit to the Peng-Robinson equation the extensive VLE data available in the literature for these high $CO_2$ and $H_2S$ mixtures. The Peng-Robinson results were consistent with APISOAVE and Ryan/Holmes as well.

The plot on the following page is an example of the comparisons we made. Figure 4 in the Ryan/Holmes paper shows the temperature vs. composition profiles for a demethanizer column with n-butane added to the condenser to prevent freezing. In this case, a 2.4% $CO_2$ overhead product was specified and the additive ratio was 8 moles/100 moles feed. The column pressure was 600 psia and the feed composion was:

| | |
|---|---|
| nitrogen | 4.8% |
| methane | 25.7% |
| carbon dioxide | 50.0% |
| ethane | 19.5% |

As can be seen, the T-X curves match quite closely. If you would like to review these comparisons in more detail, please call Bill Hensley at (713) 627-8945.

DEMETHANIZER COLUMN PROFILE COMPARISON



## Peng-Robinson Data Base

We have recently completed work on building a data base of Peng-Robinson binary interaction parameters. This data base has been installed in DESIGN/2000 and is accessed automatically then you enter the command:

BINary interaction PARameters = PENG1

in the GENeral section of your input file. The parameter PENG1 indicates it is version 1 of this data base. We will continue to update this system and these updates will be accessible using this version number. However, older versions of the data base will continue to exist and can be accessed with the appropriate version number.

This data base contains binary interaction parameters for about 170 pairs of chemicals. It covers many of the common data needs such as $CO_2$ $H_2S$, and $N_2$ in natural gas mixtures as well as some systems like $CO_2$ or $H_2S$ with water. Table 1 below provides a list of all chemical pairs for which binary interaction parameters exist.

TABLE 1

PAIRS OF CHEMICAL WHICH HAVE PENG-ROBINSON BINARY INTERACTION PARAMETERS STORED IN THE PENG1 DATA BASE

| CHEM SHARE NO. | NAME COMPONENT 1 | CHEM SHARE NO. | NAME COMPONENT 2 |
|---|---|---|---|
| 1002 | ACETONE | 3 | ETHANE |
| 65 | ACETYLENE | 22 | ETHYLENE |
| 63 | AMMONIA | 1171 | ARGON |
| | | 46 | NITROGEN |
| | | 62 | WATER |
| 3004 | AMYL ALCOHOL | 54 | 2,2-DIMETHYLBUTANE |
| | | 55 | 2,3-DIMETHYLBUTANE |
| | | 10 | N-HEXANE |
| | | 52 | 2-METHYLPENTANE |
| | | 53 | 3-METHYLPENTANE |
| 1171 | ARGON | 63 | AMMONIA |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 47 | OXYGEN |
| 40 | BENZENE | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 11 | N-HEPTANE |
| | | 5002 | HEXAFLUOROBENZENE |
| | | 10 | N-HEXANE |
| | | 2 | METHANE |
| | | 12 | N-OCTANE |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| 28 | 1,3-BUTADIENE | 6 | N-BUTANE |
| | | 24 | 1-BUTENE |
| 6 | N-BUTANE | 28 | 1,3-BUTADIENE |
| | | 24 | 1-BUTENE |
| | | 49 | CARBON DIOXIDE |
| | | 14 | N-DECANE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 5 | ISOBUTANE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| 24 | 1-BUTENE | 28 | 1,3-BUTADIENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 23 | PROPYLENE |
| 49 | CARBON DIOXIDE | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 24 | 1-BUTENE |
| | | 38 | CYCLOHEXANE |
| | | 14 | N-DECANE |
| | | 1176 | DICHLORODIFLUOROMETHANE |
| | | 1005 | DIETHYL ETHER |
| | | 3047 | DIFLUOROMETHANE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 50 | HYDROGEN SULFIDE |
| | | 5 | ISOBUTANE |
| | | 7 | ISOPENTANE |
| | | 2 | METHANE |
| | | 1021 | METHANOL |
| | | 2003 | METHYL ACETATE |
| | | 46 | NITROGEN |
| | | 1043 | NITROUS OXIDE |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| | | 23 | PROPYLENE |
| | | 41 | TOLUENE |
| | | 62 | WATER |

TABLE 1 (CONTINUED)

PAIRS OF CHEMICAL WHICH HAVE PENG-ROBINSON BINARY INTERACTION PARAMETERS STORED IN THE PENG1 DATA BASE

| CHEM SHARE NO. | NAME COMPONENT 1 | CHEM SHARE NO. | NAME COMPONENT 2 |
|---|---|---|---|
| 48 | CARBON MONOXIDE | 3 | ETHANE |
| | | 1 | HYDROGEN |
| | | 50 | HYDROGEN SULFIDE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| 1052 | CARBON TETRAFLUORIDE | 1114 | TRIFLUOROMETHANE |
| 1087 | CARBONYL SULFIDE | 2 | METHANE |
| | | 4 | PROPANE |
| 1154 | CHLORODIFLUOROMETHANE | 1122 | CHLOROPENTAFLUOROETHANE |
| | | 1176 | DICHLORODIFLUOROMETHANE |
| 1122 | CHLOROPENTAFLUOROETHANE | 1154 | CHLORODIFLUOROMETHANE |
| 1155 | CHLOROTRIFLUOROMETHANE | 1176 | DICHLORODIFLUOROMETHANE |
| | | 1114 | TRIFLUOROMETHANE |
| 1036 | M-CRESOL | 2 | METHANE |
| 38 | CYCLOHEXANE | 49 | CARBON DIOXIDE |
| | | 1072 | CYCLOHEXANONE |
| | | 7043 | CYCLOHEXENE |
| | | 1028 | 1,2-DICHLOROETHANE |
| | | 3 | ETHANE |
| | | 10 | N-HEXANE |
| | | 2 | METHANE |
| | | 8 | N-PENTANE |
| 1072 | CYCLOHEXANONE | 38 | CYCLOHEXANE |
| 7043 | CYCLOHEXENE | 38 | CYCLOHEXANE |
| | | 1028 | 1,2-DICHLOROETHANE |
| 14 | N-DECANE | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 2 | METHANE |
| 1176 | DICHLORODIFLUOROMETHANE | 49 | CARBON DIOXIDE |
| | | 1154 | CHLORODIFLUOROMETHANE |
| | | 1155 | CHLOROTRIFLUOROMETHANE |
| | | 46 | NITROGEN |
| 1028 | 1,2-DICHLOROETHANE | 38 | CYCLOHEXANE |
| | | 7043 | CYCLOHEXENE |
| 1005 | DIETHYL ETHER | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| 3047 | DIFLUOROMETHANE | 49 | CARBON DIOXIDE |
| 54 | 2,2-DIMETHYLBUTANE | 3004 | AMYL ALCOHOL |
| 55 | 2,3-DIMETHYLBUTANE | 3004 | AMYL ALCOHOL |
| 4178 | DIPHENYLMETHANE | 2 | METHANE |
| 3 | ETHANE | 1002 | ACETONE |
| | | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 38 | CYCLOHEXANE |
| | | 14 | N-DECANE |
| | | 1005 | DIETHYL ETHER |
| | | 22 | ETHYLENE |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 50 | HYDROGEN SULFIDE |
| | | 5 | ISOBUTANE |
| | | 2 | METHANE |
| | | 1021 | METHANOL |
| | | 2003 | METHYL ACETATE |
| | | 46 | NITROGEN |
| | | 12 | N-OCTANE |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| | | 23 | PROPYLENE |
| 1012 | ETHANOL | 4 | PROPANE |
| 22 | ETHYLENE | 65 | ACETYLENE |
| | | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 11 | N-HEPTANE |

TABLE 1 (CONTINUED)

PAIRS OF CHEMICAL WHICH HAVE PENG-ROBINSON BINARY INTERACTION PARAMETERS STORED IN THE PENG1 DATA BASE

| CHEM SHARE NO. | NAME COMPONENT 1 | CHEM SHARE NO. | NAME COMPONENT 2 |
|---|---|---|---|
| | | 1 | HYDROGEN |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| 1172 | HELIUM | 11 | N-HEPTANE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| 11 | N-HEPTANE | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 1172 | HELIUM |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 2 | METHANE |
| | | 8 | N-PENTANE |
| | | 1049 | 2-PENTANONE |
| | | 4 | PROPANE |
| 5002 | HEXAFLUOROBENZENE | 40 | BENZENE |
| | | 10 | N-HEXANE |
| | | 39 | METHYLCYCLOHEXANE |
| | | 41 | TOLUENE |
| 10 | N-HEXANE | 3004 | AMYL ALCOHOL |
| | | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 38 | CYCLOHEXANE |
| | | 3 | ETHANE |
| | | 11 | N-HEPTANE |
| | | 5002 | HEXAFLUOROBENZENE |
| | | 1 | HYDROGEN |
| | | 1019 | ISOPROPANOL |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| | | 3005 | TERTAMYL ALCOHOL |
| 1 | HYDROGEN | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 2 | METHANE |
| | | 3175 | 1-METHYLNAPHTHALENE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| | | 23 | PROPYLENE |
| | | 4028 | QUINOLINE |
| | | 3147 | TETRALIN |
| | | 41 | TOLUENE |
| 50 | HYDROGEN SULFIDE | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 3 | ETHANE |
| | | 5 | ISOBUTANE |
| | | 46 | NITROGEN |
| | | 62 | WATER |
| 5 | ISOBUTANE | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 50 | HYDROGEN SULFIDE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| | | 23 | PROPYLENE |
| 7 | ISOPENTANE | 49 | CARBON DIOXIDE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |

TABLE 1 (CONTINUED)

PAIRS OF CHEMICAL WHICH HAVE PENG-ROBINSON BINARY INTERACTION PARAMETERS STORED IN THE PENG1 DATA BASE

| CHEM SHARE NO. | NAME COMPONENT 1 | CHEM SHARE NO. | NAME COMPONENT 2 |
|---|---|---|---|
| 1019 | ISOPROPANOL | 10 | N-HEXANE |
| 1174 | KRYPTON | 47 | OXYGEN |
| 2 | METHANE | 1171 | ARGON |
| | | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 1087 | CARBONYL SULFIDE |
| | | 1036 | M-CRESOL |
| | | 38 | CYCLOHEXANE |
| | | 14 | N-DECANE |
| | | 4178 | DIPHENYLMETHANE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 1172 | HELIUM |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 5 | ISOBUTANE |
| | | 7 | ISOPENTANE |
| | | 3175 | 1-METHYLNAPHTHALENE |
| | | 46 | NITROGEN |
| | | 1043 | NITROUS OXIDE |
| | | 13 | N-NONANE |
| | | 12 | N-OCTANE |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| | | 3147 | TETRALIN |
| | | 41 | TOLUENE |
| | | 43 | M-XYLENE |
| 1021 | METHANOL | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 46 | NITROGEN |
| | | 62 | WATER |
| 2003 | METHYL ACETATE | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| 39 | METHYLCYCLOHEXANE | 5002 | HEXAFLUOROBENZENE |
| 3175 | 1-METHYLNAPHTHALENE | 1 | HYDROGEN |
| | | 2 | METHANE |
| 52 | 2-METHYLPENTANE | 3004 | AMYL ALCOHOL |
| 53 | 3-METHYLPENTANE | 3004 | AMYL ALCOHOL |
| 46 | NITROGEN | 63 | AMMONIA |
| | | 1171 | ARGON |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 1176 | DICHLORODIFLUOROMETHANE |
| | | 3 | ETHANE |
| | | 22 | ETHYLENE |
| | | 1172 | HELIUM |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 50 | HYDROGEN SULFIDE |
| | | 5 | ISOBUTANE |
| | | 7 | ISOPENTANE |
| | | 2 | METHANE |
| | | 1021 | METHANOL |
| | | 1043 | NITROUS OXIDE |
| | | 47 | OXYGEN |
| | | 8 | N-PENTANE |
| | | 4 | PROPANE |
| | | 23 | PROPYLENE |
| 1043 | NITROUS OXIDE | 49 | CARBON DIOXIDE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 47 | OXYGEN |
| 13 | N-NONANE | 2 | METHANE |
| 12 | N-OCTANE | 40 | BENZENE |
| | | 3 | ETHANE |
| | | 2 | METHANE |
| 47 | OXYGEN | 1171 | ARGON |

TABLE 1 (CONTINUED)

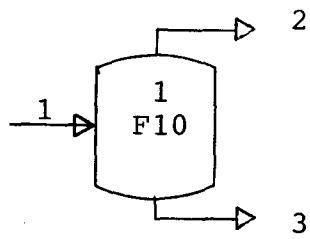
PAIRS OF CHEMICAL WHICH HAVE PENG-ROBINSON BINARY INTERACTION PARAMETERS STORED IN THE PENG1 DATA BASE

| CHEM SHARE NO. | NAME COMPONENT 1 | CHEM SHARE NO. | NAME COMPONENT 2 |
|---|---|---|---|
| | | 1174 | KRYPTON |
| | | 46 | NITROGEN |
| | | 1043 | NITROUS OXIDE |
| 8 | N-PENTANE | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 38 | CYCLOHEXANE |
| | | 3 | ETHANE |
| | | 11 | N-HEPTANE |
| | | 7 | ISOPENTANE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| 1049 | 2-PENTANONE | 11 | N-HEPTANE |
| 4 | PROPANE | 40 | BENZENE |
| | | 6 | N-BUTANE |
| | | 49 | CARBON DIOXIDE |
| | | 48 | CARBON MONOXIDE |
| | | 1087 | CARBONYL SULFIDE |
| | | 3 | ETHANE |
| | | 1012 | ETHANOL |
| | | 1172 | HELIUM |
| | | 11 | N-HEPTANE |
| | | 10 | N-HEXANE |
| | | 1 | HYDROGEN |
| | | 5 | ISOBUTANE |
| | | 7 | ISOPENTANE |
| | | 2 | METHANE |
| | | 46 | NITROGEN |
| | | 8 | N-PENTANE |
| | | 23 | PROPYLENE |
| 23 | PROPYLENE | 24 | 1-BUTENE |
| | | 49 | CARBON DIOXIDE |
| | | 3 | ETHANE |
| | | 1 | HYDROGEN |
| | | 5 | ISOBUTANE |
| | | 46 | NITROGEN |
| | | 4 | PROPANE |
| 4028 | QUINOLINE | 1 | HYDROGEN |
| 3005 | TERTAMYL ALCOHOL | 10 | N-HEXANE |
| 3051 | 1,1,2,2-TETRACHLOROETHANE | 41 | TOLUENE |
| 3147 | TETRALIN | 1 | HYDROGEN |
| | | 2 | METHANE |
| 41 | TOLUENE | 49 | CARBON DIOXIDE |
| | | 5002 | HEXAFLUOROBENZENE |
| | | 1 | HYDROGEN |
| | | 2 | METHANE |
| | | 3051 | 1,1,2,2-TETRACHLOROETHANE |
| 1114 | TRIFLUOROMETHANE | 1052 | CARBON TETRAFLUORIDE |
| | | 1155 | CHLOROTRIFLUOROMETHANE |
| 62 | WATER | 63 | AMMONIA |
| | | 49 | CARBON DIOXIDE |
| | | 50 | HYDROGEN SULFIDE |
| | | 1021 | METHANOL |
| 43 | M-XYLENE | 2 | METHANE |

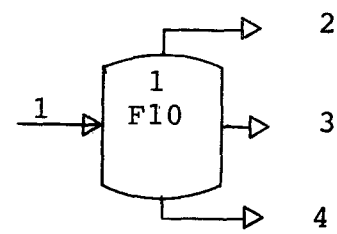
# Oil - Gas - Water Equilibrium Separator

You can now decant water from a liquid hydrocarbon stream by using the VALVE or FLASH module. All you need to do is to code three product streams out of either module, and enter IMMisible = 62 in the GENeral section. 62 is the component identification number for water. Stream 3 will contain the hydrocarbon phase and stream 4 the water phase.

With only 2 product streams the free water shows up in the liquid product, but the flowrate of the immiscible water will be reported in the detailed stream summaries. The liquid hydrocarbon stream will contain soluble water.




```
FLASH1=FL0,1,-2,-3
GENERAL
IMM=62
```




```
FLASH1=FL0,1,-2,-3,-4
GENERAL
IMM=62
```

The program calculates the solubilities of the hydrocarbons in the water steam according to reference (1) below, and then it calculates the solubility of water in the hydrocarbon stream using one of two methods. The default method for water solubility in hydrocarbons is the water in kerosene chart which is reference (2) below. Reference (3) will be used when you enter the following command in the GENeral section:

SOLubility of WATer = COMponent basis

Since solubilities are a function of carbon to hydrogen weight ratio, you can override the calculated values for petroleum fractions in reference (3), by entering in the GENeral section:

CARbon to HYDrodgen weight ratio j = value,
where j is the component ID number

The water in kerosene correlation (2) is the default correlation and is reasonable for most hydrocarbon-water systems. For light hydrocarbons (such as propane) with water, reference (3) shows significant improvement in solubility prediction.

After the phases are separated, the hydrocarbons with the soluble water becomes the second product stream, and the immiscible water with the soluble hydrocarbons becomes the third product stream. Enthalpies as well as other physical properties will be recalculated.

This feature will be available on versions 9.0 or greater.

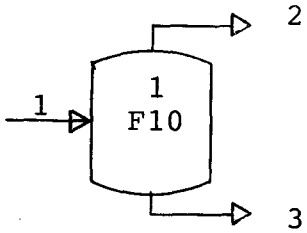
References:

(1) Calculator Programs for the Hydrocarbon Processing Industries, Vol.2, Gulf Publishing Co., p.41, (1982)
(2) API Data Book, Fig. 9A1.4, p.9-15, (1970)
(3) API Data Book, Equation 9A1.5-1, p. 9-17, (1970)

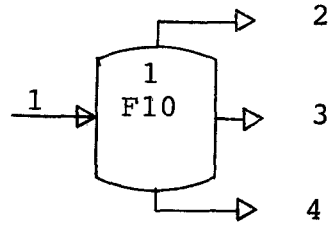
## Oil - Gas - Water Equilibrium Separator

You can now decant water from a liquid hydrocarbon stream by using the VALVE or FLASH module. All you need to do is to code three product streams out of either module, and enter IMMisible = 62 in the GENeral section. 62 is the component identification number for water. Stream 3 will contain the hydrocarbon phase and stream 4 the water phase.

With only 2 product streams the free water shows up in the liquid product, but the flowrate of the immiscible water will be reported in the detailed stream summaries. The liquid hydrocarbon stream will contain soluble water.




```
FLASH1=FL0,1,-2,-3
GENERAL
IMM=62
```




```
FLASH1=FL0,1,-2,-3,-4
GENERAL
IMM=62
```

The program calculates the solubilities of the hydrocarbons in the water steam according to reference (1) below, and then it calculates the solubility of water in the hydrocarbon stream using one of two methods. The default method for water solubility in hydrocarbons is the water in kerosene chart which is reference (2) below. Reference (3) will be used when you enter the following command in the GENeral section:

SOLubility of WATer = COMponent basis

Since solubilities are a function of carbon to hydrogen weight ratio, you can override the calculated values for petroleum fractions in reference (3), by entering in the GENeral section:

CARbon to HYDrodgen weight ratio j = value,
where j is the component ID number

The water in kerosene correlation (2) is the default correlation and is reasonable for most hydrocarbon-water systems. For light hydrocarbons (such as propane) with water, reference (3) shows significant improvement in solubility prediction.

After the phases are separated, the hydrocarbons with the soluble water becomes the second product stream, and the immiscible water with the soluble hydrocarbons becomes the third product stream. Enthalpies as well as other physical properties will be recalculated.

This feature will be available on versions 9.0 or greater.

References:

(1) Calculator Programs for the Hydrocarbon Processing Industries, Vol.2, Gulf Publishing Co., p.41, (1982)
(2) API Data Book, Fig. 9A1.4, p.9-15, (1970)
(3) API Data Book, Equation 9A1.5-1, p. 9-17, (1970)

## Oil-Water Entrainment

In addition to the equilibrium separation introduced above, non-equilibrium entrainment calculations are possible when the following commands are specified in the FLASH module:

WATer ENTrained in OIL (fraction type) = fraction of water phase entrained in the oil phase

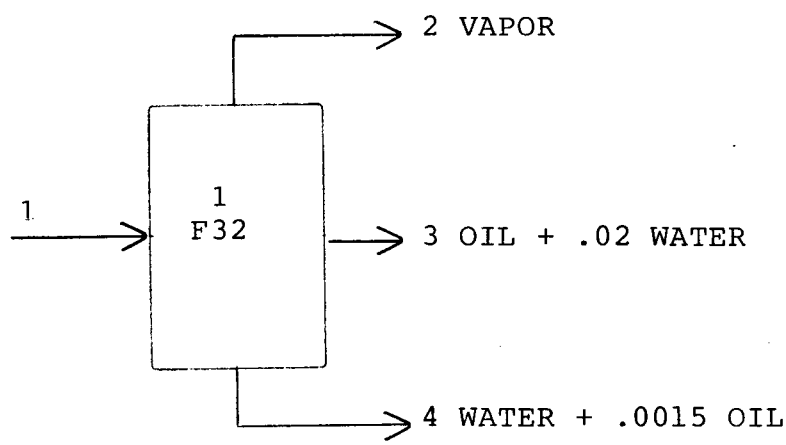
and

OIL ENTrained in WATer (fraction type) = fraction of oil entrained in water phase.

Three outlet streams must be coded when using the entrainment option.

Fraction type in these commands can be MOLar, MASs, or VOLume. MOLar is the default. The above two commands are independent of each other.

For example:




```
FLASH 1 = F32,1,-2,-4
WAT ENT OIL (VOL) =.02
OIL ENT WAT (VOL) =.0015
```

This option is available on DESIGN/2000 versions 9.0 or greater.

## Glitsch Tray Sizing

We are pleased to announce that in cooperation with Glitsch Incorporated we have added the Glitsch short-cut techniques for tower diameter calculations. You now have two choices for column sizing calculations: the Smith-Dresser-Ohlswager option previously available, or the Glitsch option. The Glitsch option allows you to either specify or calculate the percent of flood and the number of passes. In the output shown below, the tray diameters are calculated from the Glitsch procedure.

GLITSCH SHORTCUT RESULTS FOR TRAY DIAMETER, PASSES AND PERCENT FLOOD

USER-PROVIDED SPECIFICATIONS

PERCENT FLOOD = 0.00
TRAY SPACING = 0.00 IN
SYSTEM FACTOR = 0.00
NO. OF PASSES = 0.00

DEFAULT TRAY SPACING IS 24 IN IF NOT SPECIFIED. THE CORRELATION IS VALID FOR TRAY SPACINGS IN THE RANGE 12 - 48 IN.

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 | DIAMETER FT | LIQ FROM GAL/MIN | VAP TO FT3/SEC | NO. OF PASSES | PERCENT FLOOD |
|---|---|---|---|---|---|
| 1 | 2.00000 | 22.514 | 1.3600 | 1.00 | 34.67 |
| 2 | 2.00000 | 22.262 | 1.3517 | 1.00 | 34.35 |
| 3 | 2.00000 | 22.108 | 1.3458 | 1.00 | 34.15 |
| 4 | 2.00000 | 21.994 | 1.3412 | 1.00 | 34.01 |
| 5 | 2.00000 | 21.865 | 1.3368 | 1.00 | 33.86 |
| 6 | 2.00000 | 21.662 | 1.3314 | 1.00 | 33.66 |
| 7 | 2.00000 | 21.281 | 1.3233 | 1.00 | 33.29 |
| 8 | 2.00000 | 20.455 | 1.3086 | 1.00 | 32.54 |
| 9 | 2.00000 | 18.549 | 1.2777 | 1.00 | 30.83 |
| 10 | 2.25000 | 81.112 | 1.2962 | 1.00 | 37.91 |
| 11 | 2.25000 | 81.596 | 1.3042 | 1.00 | 38.34 |
| 12 | 2.25000 | 81.941 | 1.3096 | 1.00 | 38.66 |
| 13 | 2.25000 | 82.209 | 1.3136 | 1.00 | 38.90 |
| 14 | 2.25000 | 82.449 | 1.3170 | 1.00 | 39.12 |
| 15 | 2.25000 | 82.708 | 1.3207 | 1.00 | 39.36 |
| 16 | 2.25000 | 83.046 | 1.3255 | 1.00 | 39.68 |
| 17 | 2.25000 | 83.538 | 1.3325 | 1.00 | 40.15 |
| 18 | 2.25000 | 84.258 | 1.3424 | 1.00 | 40.83 |
| 19 | 2.25000 | 84.842 | 1.3491 | 1.00 | 41.42 |
| 20 | 2.25000 | 85.090 | 1.3391 | 1.00 | 41.57 |
| 21 | REBOILER | 40.208 | 0.00000 | | |

NOTE: DIAMETER IS EXPECTED TO BE WITHIN 3 IN OF GLITSCH BULLETIN 4900 DESIGN PROCEDURE FOR BALLAST TRAYS.

In the input you can set:

1. system factor
2. percent of flood
3. number of passes
4. spacing of trays

The optional commands in the DIStillation module are:

| | |
|---|---|
| GLItsch SYStem factor = | (default = 1.0) |
| GLItsch PERcent flood = | (default = determined by calculation) |
| GLItsch number of PASses = | (default = determined by calculation) |
| GLItsch SPAcing of trays (L units) = | (default = 2 ft.) |

If you specify PRISWI=2 (or greater), you will automatically get one page of output containing the Glitsch shortcut tray sizing output.

The Glitsch option is based on short-cut methods provided to ChemShare by Glitsch, and are generally within about 3 inches of the calculated results in their handbook for tray sizing. However, the results presented are not to be taken as performance guarantees. Results presented in our programs should be sent to Glitsch for rigorous calculations and guarantees that Glitsch may want to make. Address inquiries to your local Glitsch representative or send them to:

Glitsch, Inc.
P. O. Box 226227
Dallas, Texas 75266

Phone Number: (214)631-3841

This option is available on version 9.1.

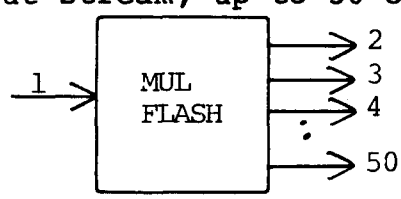
## Multiple Flash Module

A new module has been developed which performs different types of flash calculations. The module can simultaneously flash up to 50 outlet streams and can perform the following flash options:

- adiabatic flash
- isothermal flash
- isentropic flash
- adiabatic flash with addition or subtraction of heat
- bubble point temperature or pressure
- dew point temperature or pressure
- flash calculation at specified liquid molar or mass fraction
- water dew point (for separate water phase)

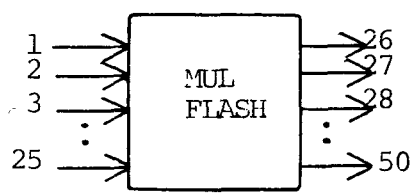
The two options graphically presented are:

1. One input stream, up to 50 outlet streams.




(all outlet streams have same composition/flowrate as inlet stream).

2. Each input stream has 1 outlet stream



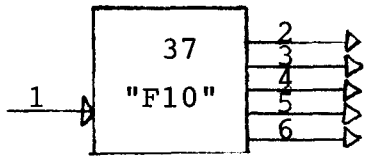

(each inlet stream has different composition/flowrates).

This module does not do phase separations. This is usually done in the FLAsh or VALve module.

This feature is available on versions 9.0 and greater.

Let's look at a couple of examples.

Example 1



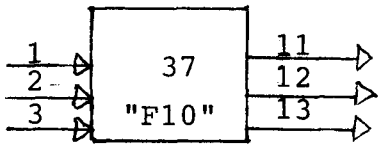

Conditions on outlet - stream 2 - bubble point temperature
stream 3 - dewpoint temprature
stream 4 - liquid to feed ratio set to .7
stream 5 - pressure out set to 30 psia
stream 6 - temperature out set at 95°C

Coding

```
MUL FLASH 37 = F10, 1,-2,-3,-4,-5,-6

BUB=2, DEW=3, LIQ FRAC=4,.7 PRE OUT=5,30, TEM OUT(C)= 6,95
```

Example 2




Conditions on outlet : stream 11 - isentropic flash
stream 12 - add 3.4 MMBTU/HR
stream 13 - make it a liquid

Coding

```
MUL FLASH37=F10,1,2,3,-11,-12,-13
ISEN=11, HEAT ADD(BTU/HR) =12,3.5E6, LIQ=13
```

Except for the isothermal flash, you can specify either TEMperature OUT or PREssure OUT, plus one other specification. The program will then solve for the corresponding pressure or temperature. If both TEM OUT and PRE OUT are specified, temperature will be varied. If no information is given for an outlet stream, the inlet conditions will be used.

This MULtiFLAsh module gives you tremendous flexibility not previously available. Remember each stream will appear in the STREAM SUMMARY and STREAM DETAILS, so all the phase properties for each stream are presented at the specified conditions.

EQUIPMENT Module Commands (j1 and j2 refer to outlet stream numbers)

ADIabatic = j1, j2, , . . .
Specify the stream numbers for adiabatic flash calculations.

BUBble point = j1, j2, , . . .
Specify the stream numbers for bubble point calculations.

DEW point = j1, j2, , . . .
Specify the stream numbers for dew point calculations (Hydrocarbon dew point for immiscible flash)

DEW WATer = j1, j2, , . . .
Specify the stream numbers for water dew point calculation (for immiscible flash only)

HEAt ADDed (H units/t units) = j1, Spec., j2, Spec, . . .
Specify the stream numbers for adiabatic flash and amount(s) of heat added or subtracted from the flash (a negative value indicates heat subtracted) in pairs.

ISEntropic = j1, j2, . . .
Specify the stream numbers for isentropic flash

LIQuid = j1, j2, . . .
Specify the outlet stream numbers to be set to liquid phase at the inlet T & P

LIQuid FRAction = j1, Spec., j2, Spec. . .
Specify the stream number(s) and the desired molar liquid fraction(s) in pairs

LIQuid FRAction (MASs) = j1, Spec., j2, Spec. . .
Specify the stream number(s) and the desired mass liquid fraction(s) in pairs

PREssure OUT (P units) = j1, Spec., j2 , Spec., . . .
Specify the stream number(s) and the desired outlet pressure(s) in pairs

TEMperature OUT (T units) = j1, Spec., j2 , Spec.
Specify the stream number(s) and the desired outlet temperature(s) in pairs

VAPor stream = j1, j2,
Specify the outlet stream numbers to be set to vapor phase at the inlet T & P

## Phase Map

A new module, PHAse MAP, has been included in DESIGN/2000 for phase envelope calculations of hydrocarbon systems. The new module uses improved numerical techniques to perform rigorous calculations around the critical region where, previously, numerical difficulties have occurred. At the present time the PHAse MAP module uses only the SOAVE equation of state for calculation. However, the calculation will still be performed using the SOAVE equation when any of the following thermo options are specified in the GENeral section: APISOAVEK, PENK, STDK, KVAL, RKK, BWRK, and BWRSK. To use the new module, specify the following commands.

```
PHA MAP1 = PHAS,1,-2
TEM BUB (T units)=
TEM DEW (T units)=
```

where the temperature of the bubble point and dew point are initial guesses.

In addition to an improved calculation of bubble and dew point curves, the module also calculates constant liquid fraction lines within the envelope. A maximum number of 5 constant liquid fraction lines is allowed. When you request this phase map, the liquid fraction line of .50 is automatically generated.

Additional commands are:

```
LIQuid FRAction                =__,__,__,__,__
TEMperature GUEss(T units)     =__,__,__,__,__
INItial PREssure(P units)      =__,__,__,__,__
```

The values entered on the right of the equal sign in each of these commands correspond. The last two commands are optional. If TEM GUE is not specified, the program will default a reasonable starting value for calculation. If INI PRE is not specified, then the calculation uses P=10 atm. as a starting pressure. The results are presented in tabular form for bubble and dew points as well as constant liquid fraction lines. The critical temperature and pressure are now printed at the beginning of the tables. Also, a plot of the envelope is included for all curves. A sample output is shown below. This is available on versions 9.0 or greater, and is on our PRIME now.

PHASE MAP USES SOAVE EQ FOR K-VALUES WITHOUT INTERACTION PARAMETERS

CRITICAL TEMPERATURE : 40.804F
CRITICAL PRESSURE : 2191.872PSIA

RESULTS FOR LIQUID FRACTION = 0.0000

| | TEMP F | PRES PSIA | Z-FACTOR | ENTHALPY BTU/LBMO |
|---|---|---|---|---|
| 1 | 198.3043 | 293.9199 | 0.95740 | 1748.3 |
| 2 | 202.2637 | 323.9984 | 0.95430 | 1778.7 |
| 3 | 206.1174 | 356.9780 | 0.95099 | 1806.0 |
| 4 | 210.2104 | 396.9112 | 0.94710 | 1832.1 |
| 5 | 214.5001 | 445.6850 | 0.94249 | 1855.3 |
| 6 | 218.9069 | 505.8105 | 0.93701 | 1873.0 |
| 7 | [illegible] | [illegible] | 0.93041 | [illegible] |

RESULTS FOR LIQUID FRACTION = 1.0000

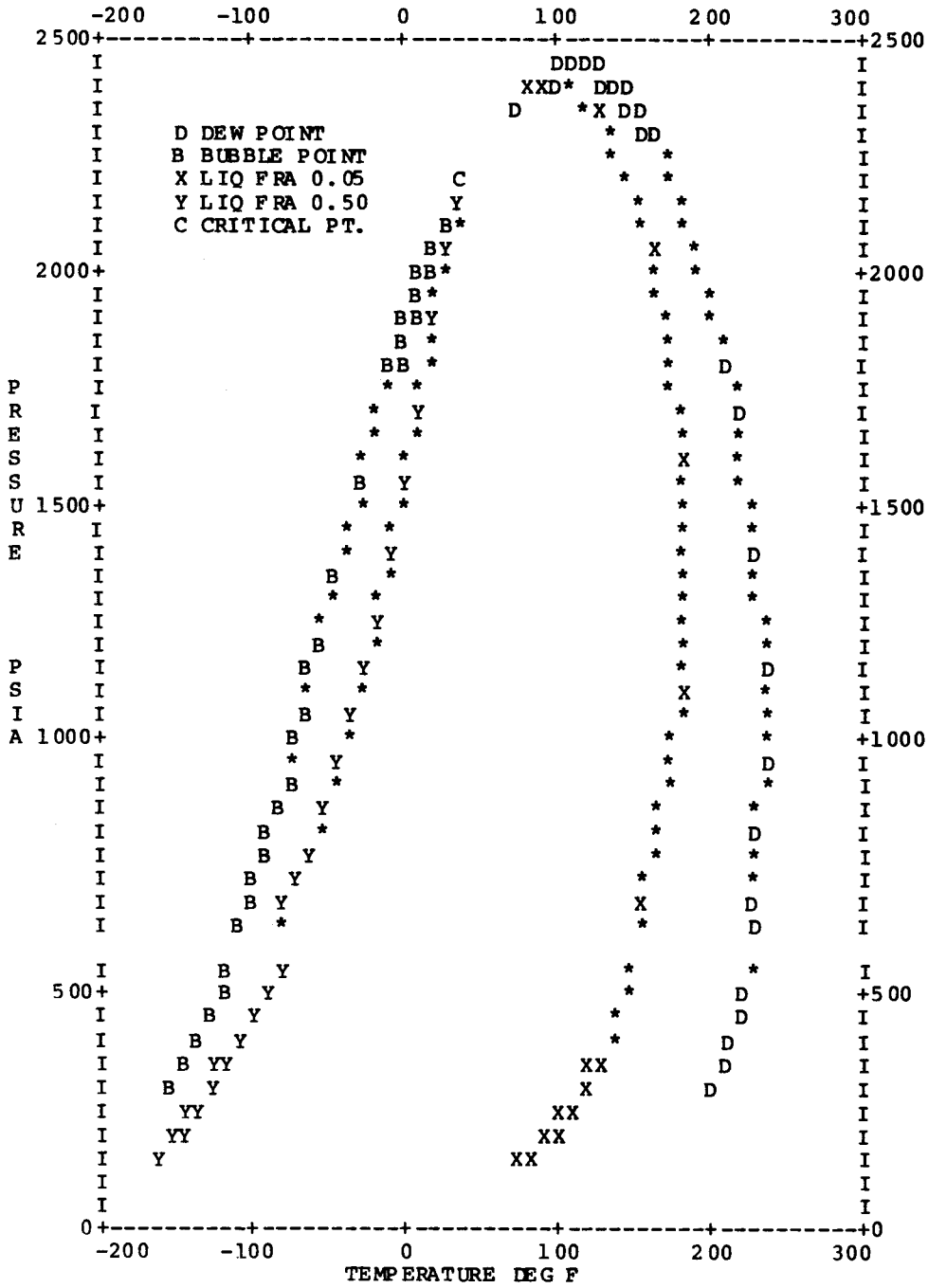
| | TEMP F | PRES PSIA | Z-FACTOR | ENTHALPY BTU/LBMO |
|---|---|---|---|---|
| 1 | -152.2015 | 293.9199 | 7.74093E-02 | -6610.9 |
| 2 | -146.6597 | 325.1846 | 8.50261E-02 | -6514.3 |
| 3 | -141.2446 | 357.7983 | 9.29453E-02 | -6419.0 |
| 4 | -135.7843 | 392.8046 | 0.10142 | -6322.0 |
| 5 | -130.2899 | 430.2338 | 0.11047 | -6223.6 |
| 6 | -124.7736 | 470.0912 | 0.12010 | -6123.9 |
| 7 | -119.2495 | 512.3523 | 0.13030 | -6023.2 |
| 8 | -113.7330 | 556.9591 | 0.14106 | [illegible] |
| 9 | [illegible] | | [illegible] | |

RESULTS FOR LIQUID FRACTION = 0.0500

| | TEMP F | PRES PSIA | Z-FACTOR VAPOR | Z-FACTOR LIQUID |
|---|---|---|---|---|
| 1 | 76.8270 | 147.0005 | 0.96679 | 6.14464E-02 |
| 2 | 81.8984 | 162.4607 | 0.96439 | 6.72223E-02 |
| 3 | 87.2974 | 180.4413 | 0.96169 | 7.38540E-02 |
| 4 | 92.7360 | 200.2848 | 0.95882 | 8.10734E-02 |
| 5 | 98.2064 | 222.1638 | 0.95577 | 8.89222E-02 |
| 6 | 103.6996 | 246.2639 | 0.95254 | 9.74439E-02 |
| 7 | 109.2053 | 272.7842 | 0.94911 | 0.10668 |
| 8 | 114.7114 | 301.9369 | 0.94548 | 0.11668 |
| 9 | 120.2042 | 333.9481 | 0.94164 | [illegible]749 |
| 10 | 125.1075 | 365.2975 | [illegible] | |
| 11 | 156.8910 | 663.5927 | | |
| 12 | 177.4886 | | | |
| 13 | [illegible] | | | |

RESULTS FOR LIQUID FRACTION = 0.5000

| | TEMP F | PRES PSIA | Z-FACTOR VAPOR | Z-FACTOR LIQUID |
|---|---|---|---|---|
| 1 | -167.9234 | 147.0005 | 0.86999 | 4.56256E-02 |
| 2 | -161.8535 | 166.5537 | 0.85931 | 5.09754E-02 |
| 3 | -155.8126 | 187.6817 | 0.84839 | 5.66780E-02 |
| 4 | -149.6022 | 211.2044 | 0.83687 | 6.29449E-02 |
| 5 | -143.2216 | 237.3456 | 0.82475 | 6.98226E-02 |
| 6 | -136.6706 | 266.3425 | 0.81202 | [illegible] |
| 7 | -129.[illegible] | | | |


D DEW POINT
B BUBBLE POINT
X LIQ FRA 0.05
Y LIQ FRA 0.50
C CRITICAL PT.
PRESSURE PSIA
TEMPERATURE DEG F
-200
-100
0
100
200
300
2500
2000
1500
1000
500
0

## Heating and Cooling Curves

You can now have heating and cooling curves calculated without using the HEAt EXChanger module. This will allow you to get curves for the rigorous distillation condenser and reboiler as well as any stream in the flowsheet. The output, as shown below, includes the plotted results of the tabular data. This feature is implemented on version 9.0 or later, and is available to users on our PRIME computer systems now.

**The new commands are:**

**A. In the rigorous distillation unit (DIS)**

**CONdenser CURve**

**and/or**

**REBoiler CURve**

**B. For streams, add to the GENeral section**

**HEAt CURve i**

**and/or**

**COOL CURve i**

**where i = stream number**

With either of these 2 commands in the GENeral section, you will automatically get 10 increments from the stream temperature to the bubble or dew point with no pressure drop. To modify any of these options, the command in its full form is:

```
          COOL CURve (T units, P units) i = x,y,z
          HEAt CURve (T units, P units) i = x,y,z
where       i = stream number
            x = delta T (or specify BUB or DEW)
            y = delta P
            z = number of increments
```

For example:

COOL CURve 12 = 250, 40.3, 15

This will generate a cooling curve with a delta T of 250 degrees F from the temperature of stream 12 with a pressure drop of 40.3 psi distributed equally across the 15 increment curve.

An example of the output using the COND CURve command on the distillation column is shown below. This is one feature which was added as a result of customers' requests. If there are other options or features you would like to see in the programs, please let us know.

+++ COOLING CURVE +++
TOTAL FLOW RATE = 658.51 LBMOL/HR

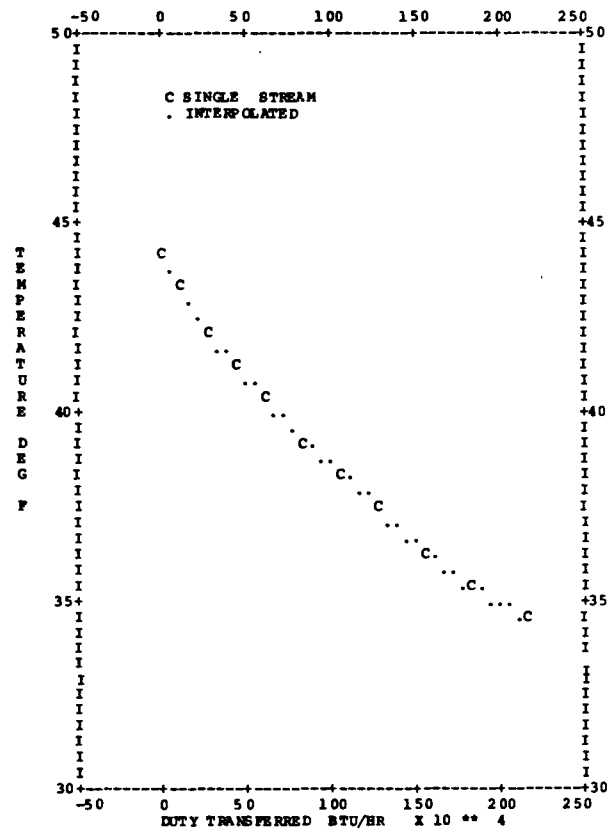
| | TEMPERATURE F | PRESSURE PSIA | LIQUID FLOW LBMOL/HR | LIQUID FLOW LB/HR | MOLECULAR WEIGHT LIQUID | MOLECULAR WEIGHT VAPOR |
|---|---|---|---|---|---|---|
| 1 | 44.11 | 345.00 | 0.00 | 0.00 | 0.00 | 30.91 |
| 2 | 43.15 | 344.50 | 30.03 | 969.19 | 32.28 | 30.85 |
| 3 | 42.18 | 344.00 | 62.99 | 2024.82 | 32.15 | 30.78 |
| 4 | 41.22 | 343.50 | 99.35 | 3180.61 | 32.01 | 30.72 |
| 5 | 40.25 | 343.00 | 139.77 | 4456.02 | 31.88 | 30.65 |
| 6 | 39.29 | 342.50 | 184.94 | 5871.53 | 31.75 | 30.59 |
| 7 | 38.32 | 342.00 | 235.64 | 7450.28 | 31.62 | 30.52 |
| 8 | 37.36 | 341.50 | 292.50 | 9210.56 | 31.49 | 30.45 |
| 9 | 36.40 | 341.00 | 355.60 | 11153.27 | 31.36 | 30.38 |
| 10 | 35.43 | 340.50 | 423.82 | 13243.62 | 31.25 | 30.31 |
| 11 | 34.47 | 340.00 | 493.91 | 15381.14 | 31.14 | 30.22 |

COOLING CURVE (CONTINUED)

| | DENSITY LB/FT3 LIQUID | DENSITY LB/FT3 VAPOR | ENTHALPY BTU/HR LIQUID | ENTHALPY BTU/HR VAPOR | COOLING DUTY BTU/HR |
|---|---|---|---|---|---|
| 1 | 0.00 | 2.75 | 0. | -447742. | 0. |
| 2 | 25.45 | 2.75 | -149332. | -434219. | 135810. |
| 3 | 25.42 | 2.74 | -313303. | -417937. | 283499. |
| 4 | 25.38 | 2.74 | -494222. | -398469. | 444949. |
| 5 | 25.35 | 2.73 | -695257. | -375240. | 622755. |
| 6 | 25.32 | 2.73 | -919923. | -347598. | 819779. |
| 7 | 25.28 | 2.73 | -1172134. | -314806. | 1039198. |
| 8 | 25.25 | 2.72 | -1455011. | -276223. | 1283492. |
| 9 | 25.22 | 2.72 | -1769224. | -231595. | 1553077. |
| 10 | 25.20 | 2.71 | -2109434. | -181638. | 1843330. |
| 11 | 25.18 | 2.70 | -2460088. | -128807. | 2141154. |

| PRESSURE, PSIA | BUBBLE POINT, F | DEW POINT, F |
|---|---|---|
| 345.00 | 33.146 | 44.111 |
| 340.00 | 32.014 | 43.081 |

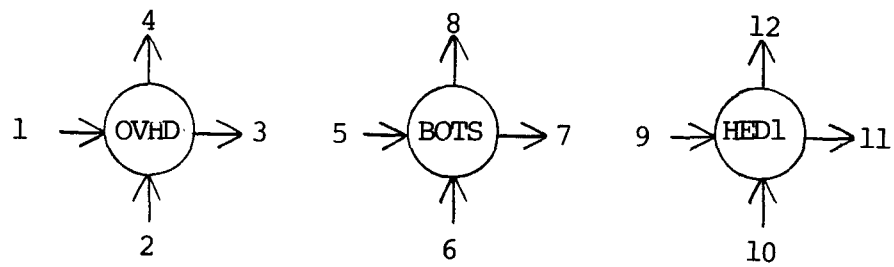
COOLING CURVE (CONTINUED)



## Simplified Input on Feed Streams

If you have a flowsheet in which the same stream composition and/or conditions are being used in several places, you can use this new feature to avoid typing in the stream data numerous times.

For example:




Streams: 1,5 and 9 have the same FLOWs and T,P
Streams: 2,6, and 10 have the same FLOWs and T,P

```
* COPIED STREAMS
HEA EXC1=OVHD, 1 ,2 ,-3 ,-4,TEM APP=10
HEA EXC2=BOTS, 5, 6, -7, -8,TEM APP=20
HEA EXC3=HED1, 9,10,-11,-12,TEM APP=40
GEN,
  COM=4,5,6,7,8,10,11
  TP(C,MMHG)1=80,210
  FLO(LB/HR)1=2000,400,600,150,200,51,250
  TP(C,MMHG)2=40,169
  FLO(LB/HR)2=70,90,350,5,180,650,20
  TP5=TP1
  FLO(LB/HR)5=FLO1
  TP6=TP2
  FLO(LB/HR)6=FLO(LB/HR)2
  TP(C,MMHG)9=TP(C,MMHG)1
  FLO9=FLO1
  TP10=TP2
  FLO10=FLO2

END
```

For streams which have the same flow (inlet, recycle) you don't have to retype all the information. Just tell the program which stream has the same flow. The same can be done for the TP information. The TP copy stream does not have to be the same as the flow copy stream. The example above illustrates that input units are not needed on the copy-stream commands, and have no effect if they appear.

This option is available on versions 9.0 or later.

## Feeds To The Distillation Column

We have added a feature to the rigorous distillation unit which allows you to specify that a feed is at its bubble point, dew point or at a specific liquid to feed ratio. The resultant temperature is printed in the feed flash summary before the column calculation. To use any of these features simply add any of the following commands to the DIStillation equipment input:

```
BUBble point = j1,j2,. . .
DEW point    = j
LOF          = fraction, or      = fraction,fraction,...
                                   (for each feed in top
VAPor        = j                    to bottom order)
LIQuid       = j
```

where j is the stream number of the feed stream. The LOF (liquid to feed ratio) values are entered in the same order as the LOCation of FEEds command. A zero value of LOF causes that stream to be treated in the normal fashion ie - it will be flashed from the temperature and pressure given for the feed to the tray pressure. The phase of a feed can also be forced with a LIQ or VAP command. For example, to set a bubble point temperature on feed 1 and dewpoint temperature for feed 2, the commands are:

```
DIS5=CONT,17,24-3,-4,ABS
TRA=7,LOCFEE=1,8,
BUB=17,DEW=24
```

## Separator Sizing

We are now able to offer preliminary vessel sizing calculations for flash drums and accumulators performing single stage liquid-vapor separation. This is the second in a series of sizing capabilities which allow the process engineer to size equipment in his flowsheet simulation.

The separator vessel corresponds to either a FLAsh drum or a VALve module on the DESIGN/2000 flowsheet and can be sized as either a vertical or horizontal vessel. Flexible input specifications are available with reasonable defaults supplied for values not specified. Output contains relevant process and mechanical information. For vertical vessels, a scaled vessel layout showing dimensions and nozzle locations is also provided.

A simple example of input and output is shown below:

```
*EXAMPLE OF VERTICAL SEPARATOR SIZING
FLASH DRUM 19 = S306,16,-11,-44,VERTICAL
GENERAL
COMPONENTS = 2,3,4
FLOW 16=800,100,100
TP16 = -45,290
END
```

****** SEPARATOR SIZING RESULTS FOR VERTICAL SEPARATOR 19 *******
VAPOR STREAM = 11 LIQUID STREAM = 44
NOTE: K-CONSTANT FROM FLUID PROPERTIES = 0.44 FT/SEC

CONDITIONS

| | | | |
|---|---|---|---|
| LIQUID FLOW RATE | T-P | 1.9917 | GAL/MIN |
| VAPOR FLOW RATE | T-P | 200.73 | FT3/MIN |
| TOTAL FLOW RATE | T-P | 202.72 | FT3/MIN |
| TEMPERATURE | | -45.000 | DEG F |
| PRESSURE | | 290.00 | PSIA |

PROPERTIES

| | | | |
|---|---|---|---|
| DENSITY | VAPOR | 1.3722 | LB/FT3 |
| DENSITY | LIQUID | 31.152 | LB/FT3 |
| DENSITY | MIXED | 1.6648 | LB/FT3 |
| Z-FACTOR | VAPOR | 0.88022 | |

DESIGN PARAMETERS

| | | | |
|---|---|---|---|
| K CONSTANT | DEFAULT | 0.35000 | FT/SEC |
| MIN DISENGAGING HEIGHT | DEFAULT | 3.0000 | FT |
| MIN LIQ TO INLET HEIGHT | DEFAULT | 2.0000 | FT |
| MIN LEVEL NOZZLE HEIGHT | DEFAULT | 1.5000 | FT |
| MIST ELIMINATOR | DEFAULT | 0.50000 | FT |
| DESIGN PRESSURE | DEFAULT | 319.00 | PSIA |
| ALLOWABLE STRESS | DEFAULT | 15015. | PSIA |
| JOINT EFFICIENCY | DEFAULT | 1.0000 | |
| CORROSION ALLOWANCE | DEFAULT | 0.12500 | IN. |
| WEIGHT PERCENT ALLOWANCE | DEFAULT | 20.000 | |

RESULTS

| | | |
|---|---|---|
| ALLOWABLE VAPOR VELOCITY | 1.6305 | FT/SEC |
| ACTUAL VAPOR VELOCITY | 1.1347 | FT/SEC |
| DIAMETER BASED ON SEPARATION | 1.6243 | FT |
| SUITABLE DIAMETER USING PIPE I.D. | 23.250 | IN. |
| PIPE NOMINAL DIAMETER | 24.000 | IN. |
| SUITABLE LENGTH | 8.0000 | FT |
| SURGE TIME TO HLL | 17.764 | MIN |
| HIGH LIQUID LEVEL (HLL) HEIGHT | 1.5000 | FT |
| HLL TO INLET HEIGHT | 3.0000 | FT |
| DISENGAGING HEIGHT | 3.0000 | FT |
| WALL THICKNESS (STD ) | 0.37500 | IN. |
| MIN SHELL THICKNESS | 0.25047 | IN. |
| MIN HEAD THICKNESS | 0.24781 | IN. |
| APPROX WEIGHT OF STEEL VESSEL(EMPTY) | 532.82 | LB |
| APPROX WEIGHT OF VESSEL (FULL) | 1267.6 | LB |
| APPROX TOTAL WEIGHT INCL. ALLOWANCE | 1907.0 | LB |
| INSULATION MAY BE NEEDED SINCE TEMP = | -45.000 | DEG F |

****** SEPARATOR SIZING RESULTS FOR VERT SEPARATOR 19 **********

| NOZZLES | A INLET | B VAP OUT | C LIQ OUT | |
|---|---|---|---|---|
| MINIMUM VELOCITY | 46.502 | 51.220 | 10.750 | FT/SEC |
| ACTUAL VELOCITY | 68.875 | 68.198 | 6.0900 | FT/SEC |
| MAXIMUM VELOCITY | 77.503 | 85.366 | 17.917 | FT/SEC |
| DIAMETER (O.D.) | 3.0000 | 3.0000 | 1.0000 | IN. |

NOTE: MINIMUM NOZZLE DIAMETER IS SELECTED

**** SKETCH OF VERTICAL FLASH DRUM 19 (TO APPROX.SCALE ONLY) ****

```
                    === B
                     I
                    ***
                 ****   ****
               **            **
              I+++++++++++++++I       -
              I   MIST PAD    I       I
        -     I+++++++++++++++I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
   3.00 FT    I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I       I
        I     I               I     6.50 FT
        I  I  I               I       I
        -  I==I               I       I
           I  I               I       I
              I               I       I
           A  I               I       I
              I               I       I
              I               I       I
              I               I       I
              I               I       I
              I               I       I
              I               I       I
              I               I       I
              I               I       I
              I    VAPOR      I       I
              I               I  I    I
              I-----HLL-------I==I    -
              I               I  I    I
              I    LIQUID     I       I
              I               I       I
              I               I     1.50 FT
              I               I       I
              I               I  I    I
              I               I==I    -
               **            **   I
                 ****   ****
                    *I*
                    === C

               --   1.93 FT---
```

## Line Sizing

The line sizing capability announced in the May '82 newsletter has been further enhanced to allow you to make many different specifications. This is now available in DESIGN/2000 version 9.0.

The following sample sizes one horizontal two-phase line and one vertical gas line to meet your maximum velocity specifications.

```
SIZE LINES
USE STREAMS = 1,3
DIRECTION OF FLOW = HORIZONTAL,UP
MAXIMUM VELOCITY (FT/SEC) = 20,10
PIPE SIZE CODE = 2*XXS
```

These commands form a "sizing section" which can be coded anywhere in your input file, just like the GENeral section.

Three pipe sizes are reported for each line: T represents the target size (i.e. smallest which satisfies your specification). Flow conditions for one size larger (L) and smaller (S) are also reported for comparison. In the two phase case the proximity to flow regime boundaries is illustrated on the Baker chart for each of the three sizes.

********** LINE SIZING RESULTS FOR 2 PHASE STREAM 1 **********

USING METHOD OF LOCKHART-MARTINELLI
ASSUMING ISOTHERMAL FLOW IN HORIZONTAL DIRECTION

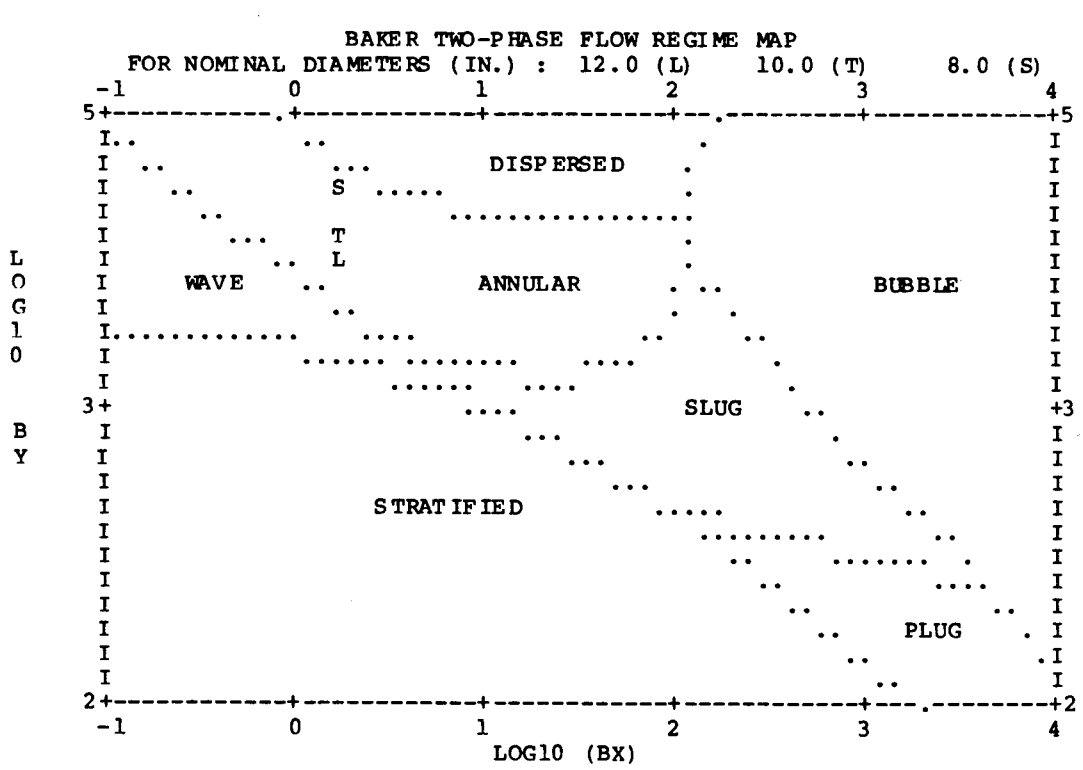
| | | |
|---|---|---|
| VAPOR FLOW RATE | LB/HR | 0.3205E 05 |
| LIQUID FLOW RATE | LB/HR | 3303. |
| LIQUID VOLUME FRACTION | | 0.3593E-02 |
| TEMPERATURE | DEG F | 93.00 |
| INLET PRESSURE | PSIA | 150.0 |
| MAX VELOCITY SPEC | FT/SEC | 20.00 |
| LINE LENGTH | FT | 100.0 |
| ELEVATION | FT | 0.0000 |
| PIPE SCHEDULE | | XXS |

| | | | |
|---|---|---|---|
| DENSITY - | VAPOR | 1.170 | LB/FT3 |
| | LIQUID | 33.45 | LB/FT3 |
| MOLECULAR WEIGHT - | VAPOR | 40.87 | |
| | LIQUID | 54.42 | |
| VISCOSITY - | VAPOR | 0.9840E-02 | CP |
| | LIQUID | 0.1058 | CP |
| Z-FACTOR | | 0.8834 | |
| SURFACE TENSION | | 8.648 | DYNES/CM |

* * * * * * * * * * * * * * * * * * * * * * * *

| | | LARGER | TARGET | SMALLER |
|---|---|---|---|---|
| I.D. FOR BAKER MAP | | L | T | S |
| NOMINAL DIAMETER | IN. | 12.00 | 10.00 | 8.000 |
| INTERNAL DIAMETER | IN. | 10.75 | 8.750 | 6.875 |
| DELTA P (FRICTION) | PSIA | 0.2528E-01 | 0.1091 | 0.4599 |
| DELTA P (ELEVATION) | PSIA | 0.0000 | 0.0000 | 0.0000 |
| DELTA P (TOTAL) | PSIA | 0.2528E-01 | 0.1091 | 0.4599 |
| MEETS VELOCITY SPEC | | YES | YES | NO |
| OUTLET PRESSURE | PSIA | 150.0 | 149.9 | 149.5 |
| LIQUID VELOCITY | FT/SEC | 0.4353E-01 | 0.6570E-01 | 0.1064 |
| VAPOR VELOCITY | FT/SEC | 12.07 | 18.22 | 29.52 |
| 2-PHASE VELOCITY | FT/SEC | 0.0000 | 0.0000 | 0.0000 |
| NO SLIP VELOCITY | FT/SEC | 12.12 | 18.29 | 29.62 |
| REYNOLDS NUMBER | VAPOR | 0.1912E 07 | 0.2349E 07 | 0.2990E 07 |
| REYNOLDS NUMBER | LIQUID | 0.1832E 05 | 0.2251E 05 | 0.2865E 05 |
| FROUDE NUMBER | | 5.093 | 14.25 | 47.60 |
| FLOW REGIME - BAKER | | ANNULAR | ANNULAR | ANNULAR |
| FRICTION FACTOR | VAPOR | 0.1385E-01 | 0.1424E-01 | 0.1480E-01 |
| FRICTION FACTOR | LIQUID | 0.2680E-01 | 0.2562E-01 | 0.2442E-01 |
| 2-PHASE DENSITY | LB/FT3 | 4.547 | 4.080 | 3.518 |
| LIQUID HOLDUP | | 0.1046 | 0.9016E-01 | 0.7274E-01 |

********** LINE SIZING RESULTS FOR 2 PHASE STREAM 1 **********




********** LINE SIZING RESULTS FOR GAS STREAM 3 **********

USING METHOD OF DARCY
ASSUMING ISOTHERMAL FLOW IN VERTICAL (UP) DIRECTION

| | | |
|---|---|---|
| VAPOR FLOW RATE | LB/HR | 0.6587E 05 |
| TEMPERATURE | DEG F | 45.00 |
| INLET PRESSURE | PSIA | 655.0 |
| MAX VELOCITY SPEC | FT/SEC | 10.00 |
| LINE LENGTH | FT | 100.0 |
| ELEVATION | FT | 100.0 |
| PIPE SCHEDULE | | XXS |

| | | | | |
|---|---|---|---|---|
| DENSITY | - | VAPOR | 7.976 | LB/FT3 |
| MOLECULAR WEIGHT | - | VAPOR | 41.80 | |
| VISCOSITY | - | VAPOR | 0.1638E-01 | CP |
| Z-FACTOR | | | 0.6337 | |

* * * * * * * * * * * * * * * * * * * * * * * *

| | | LARGER | TARGET | SMALLER |
|---|---|---|---|---|
| NOMINAL DIAMETER | IN. | 10.00 | 8.000 | 6.000 |
| INTERNAL DIAMETER | IN. | 8.750 | 6.875 | 4.897 |
| DELTA P (FRICTION) | PSIA | 5.046 | 17.55 | 102.1 |
| DELTA P (ELEVATION) | PSIA | 5.539 | 5.539 | 5.539 |
| DELTA P (TOTAL) | PSIA | 10.59 | 23.09 | 107.6 |
| MEETS VELOCITY SPEC | | YES | YES | NO |
| OUTLET PRESSURE | PSIA | 644.4 | 631.9 | 547.4 |
| FLUID VELOCITY | FT/SEC | 5.493 | 8.898 | 17.54 |
| REYNOLDS NUMBER | | 0.2902E 07 | 0.3693E 07 | 0.5185E 07 |
| FLOW REGIME - | | TURBULENT | TURBULENT | TURBULENT |
| FRICTION FACTOR | | 0.1416E-01 | 0.1475E-01 | 0.1573E-01 |

## Transmission Lines in DESIGN/2000

The transmission LINE module is now available in DESIGN/2000 in addition to the existing line sizing capability. The LINE module can be connected to any other equipment modules in a flowsheet, such as separators and compressors, in order to simulate a long transmission line. Simple networks or gathering systems consisting of several lines can also be modelled. Lines can be gas, liquid or two-phase and phase change is detected if it occurs. Pressure drop and flow regime are predicted along the line and the resulting outlet pressure is used in downstream calculations. The calculation methods used are the same as for line sizing and are principally applicable to hydrocarbon or hydrocarbon and water systems.

Several line sections of different lengths and elevations can be modelled in a single LINE module. Results are tabulated for each of the node points specified along the line. Several LINE modules may be used to model a transmission line with intermediate compression and junctions as shown below. For two phase lines a Baker flow regime map is given for each LINE module to show proximity to flow regime boundaries.

Different diameter case studies can be made in a single LINE module calculation simply by specifying several diameters. Pressure and other profiles along the line can be plotted according to user specifications. Points on the curve correspond to the user's node points. Several LINE modules can be included in a single profile plot of a typical transmission line.

With the transmission line a part of DESIGN/2000, you can utilize all the flexibility of DESIGN/2000 including use of the CONTroller. For example, below we have a simplified platform, 10 miles offshore. We can now model the complete process on the platform, plus review the transmission system and make process changes based upon onshore delivery constraints.

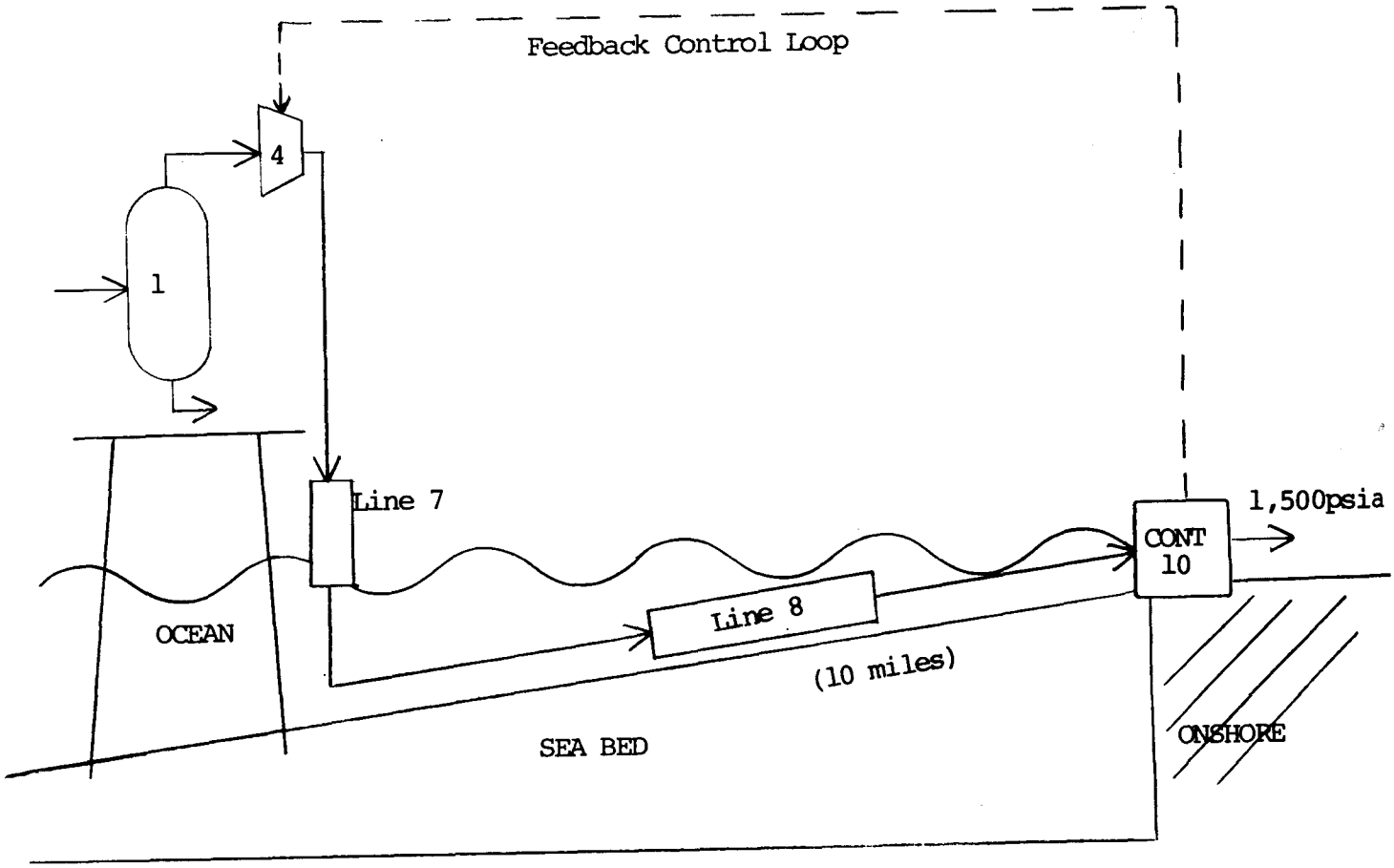
In the example below, we have a delivery pressure of 1,500 psia that must be met. We have a CONTroller monitoring the onshore pressure and adjusting the outlet pressure of the COMpressor on the platform until the delivery pressure is met.

The output includes:

1. Heat and material balance
2. Transmission lines including frictional and elevation effects
3. Separator sizing
4. Horsepower requirements
5. Graphical output of pressure and elevation profiles along the line.

Except for item 1, all the other features are unique to ChemShare's DESIGN/2000 program.

This capability is available in DESIGN/2000 version 9.0.




```
* DESIGN.OFFSHORE1      GAS LINE WITH FIXED ONSHORE PRESSURE

FLASH DRUM 1 = SEPR,1,-2,-3, VERTICAL
COMPRESSOR 4 = COMP,2,-8, ENTROPY, PRESSURE OUT = 1600
LINE 7 = LINE,8,-11, NOMINAL DIAMETER (IN) = 12, DOWN, LENGTH = 150
LINE 8 = LINE,11,-12, NOMINAL DIAMETER (IN) = 12, LENGTH (MILES) = 10*1
ELEVATION (FT) = 3*10, 5, 2, 20, 30, 3*10

CONTROLLER 10 = FIXP,12,-13, VARY PRESSURE OUT (MIN=1500,MAX=2500) OF COMPRE 4
UNTIL PRESSURE FROM STREAM 12 = 1500 (TOL=25)

GENERAL
COM = 46,49,2,3,4,5,6,7,8,10,11,12,13,14,62
IMM=62
FLOW 1 = 5,3,5000,3000,1000,700,500,233,339,226,427,207,266,234,100
TP1 = 120,1400
SOAVEK

PLOT PRESSURE AND ELEVATION AGAINST LENGTH FOR LINES = 7,8

END
```

RESULTS OF LINE 7 CALCULATION USING 12.0 IN. NOMINAL PIPE
LINE IS VERTICAL (DOWN) AND ISOTHERMAL
ELEVATIONS ARE REPORTED RELATIVE TO INLET NODE.
INSIDE DIAMETER 12.00 IN. PIPE SCHEDULE CODE STD
METHOD FOR FRICTION PRESSURE DROP IS DARCY-WEISBACH
METHOD FOR ELEVATION PRESSURE DROP IS PHASE DENSITY
PRESSURE DROPS (DELP) ARE PER 100 FT

| LINE NODE | LENGTH FT | ELEV. FT | TEMP. DEG F | DELP-FRIC PSIA | DELP-ELEV PSIA | PRESS. PSIA | VELOC. FT/SEC | LIQUID HOLDUP | FLOW REGIME |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0. | 0.0 | 170.15 | 0.8288 | -6.4773 | 1995.5 | 2.5 | 0.0000 | TURB |
| 2 | 150. | 150.0 | 170.15 | 0.8252 | -6.5062 | 2004.0 | 2.4 | 0.0000 | TURB |

RESULTS OF LINE 8 CALCULATION USING 12.0 IN. NOMINAL PIPE
LINE IS HORIZONTAL AND ISOTHERMAL
ELEVATIONS ARE REPORTED RELATIVE TO INLET NODE.
INSIDE DIAMETER 12.00 IN. PIPE SCHEDULE CODE STD
METHOD FOR FRICTION PRESSURE DROP IS DARCY-WEISBACH
METHOD FOR ELEVATION PRESSURE DROP IS PHASE DENSITY
PRESSURE DROPS (DELP) ARE PER 100 FT

| LINE NODE | LENGTH FT | ELEV. FT | TEMP. DEG F | DELP-FRIC PSIA | DELP-ELEV PSIA | PRESS. PSIA | VELOC. FT/SEC | LIQUID HOLDUP | FLOW REGIME |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0. | 0.0 | 170.15 | 0.8252 | 6.5062 | 2004.0 | 2.4 | 0.0000 | TURB |
| 2 | 5280. | 10.0 | 170.15 | 0.8443 | 6.3548 | 1959.8 | 2.5 | 0.0000 | TURB |
| 3 | 10560. | 20.0 | 170.15 | 0.8651 | 6.1981 | 1914.6 | 2.6 | 0.0000 | TURB |
| 4 | 15840. | 30.0 | 170.15 | 0.8878 | 6.0359 | 1868.3 | 2.6 | 0.0000 | TURB |
| 5 | 21120. | 35.0 | 170.15 | 0.9124 | 5.8689 | 1821.1 | 2.7 | 0.0000 | TURB |
| 6 | 26400. | 37.0 | 170.15 | 0.9394 | 5.6964 | 1772.8 | 2.8 | 0.0000 | TURB |
| 7 | 31680. | 57.0 | 170.15 | 0.9699 | 5.5136 | 1722.1 | 2.9 | 0.0000 | TURB |
| 8 | 36960. | 87.0 | 170.15 | 1.0041 | 5.3218 | 1669.2 | 3.0 | 0.0000 | TURB |
| 9 | 42240. | 97.0 | 170.15 | 1.0416 | 5.1265 | 1615.6 | 3.1 | 0.0000 | TURB |
| 10 | 47520. | 107.0 | 170.15 | 1.0839 | 4.9232 | 1560.1 | 3.2 | 0.0000 | TURB |
| 11 | 52800. | 117.0 | 170.15 | 1.1318 | 4.7115 | 1502.4 | 3.4 | 0.0000 | TURB |

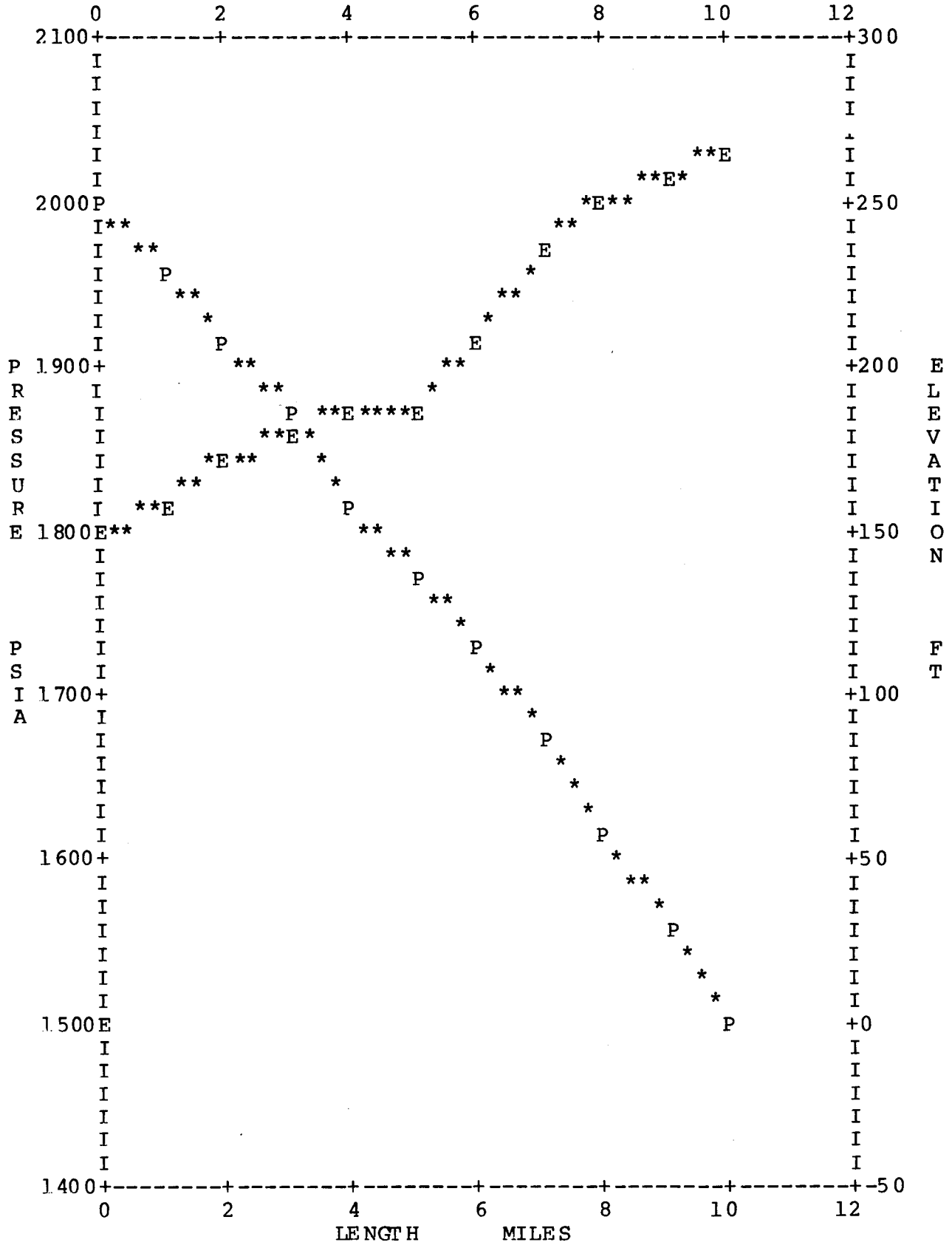
****PUMP/COMPRESSOR/EXPD****

EQUIPMENT NO. 4

EXTERNAL NAME COMP
COMP. STAGES 1.000
WORK CAPACITY
HP 0.1000E 07
OUTLET PRES.
PSIA 1996.
TYPE ENTROPY
THERMAL EFFIC. 0.6500
(OR POLYTROPIC COEFF.)
FUEL SCF/HR 4083.
REAL WORK HP 500.2
WORK IS NEGATIVE FOR EXPANDER
CP/CV 1.241

.....

LINE PLOT 1 OF PRESSURE AND ELEVATION AGAINST LENGTH

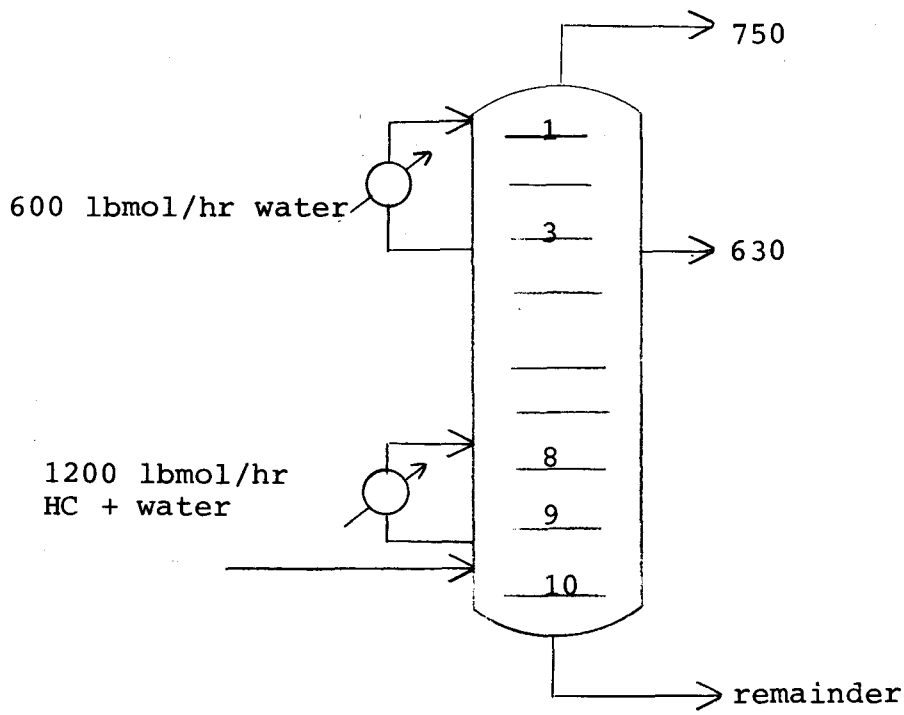


## Quench Columns

We have now added to REFINE versions 9.0 and greater, the ability to model quench columns where free water can form along with a liquid hydrocarbon and vapor on any tray in the column.

Only a few simple commands are needed to use it. This example describes the commands for this feature.

Simplified quench or water wash column




```
LOC SIDE DRAW WATER = 3
LOC SIDE DRAW       = 3  (needed if LOC SID WAT used)
PRODUCT             = 750,630,0
LOC PUMP            = 3,1,9,8
LOC PUMP WATER      = 1,0  (1 if water, 0 if HC)
PROD PUMP           = 600, 1200(lbmol/hr. HC and water)
P-S                 = .98,.99,.98,7*0 (optional but recommended for
                      estimate of the mole fraction of water
                      on each tray)
```

Some interesting points are:

1. You can decant water on any tray
2. You can have as many decants as needed
3. The pumparound can be pure water
4. We do not need coolers on each tray as SIMSCI does to create dummy pumparound affects

## Simplified Product Specifications on Refine

REFINE is the only major rigorous heat and material balance simulation program that can meet a rigorous product specification on an ASTM or TBP basis. In order to set these specifications on the rigorous runs, the coding convention was 18.XXX for ASTM and 17.XXX for TBP such as;

PROSPEC = 380, 18.095, 2, 3, 580, 17.090, 3, 4

The above command specifies: an ASTM 95% of 380°F on product 2 by varying product 3 and a TBP 90% of 580°F on product 3 by varying product 4

To simplying this coding it is now possible to use ASTM or TBP directly as follows:

PRO SPEC = 480,ASTM95,2,3,580,TBP90,3,4

This feature is available on REFINE versions 9.0 and later.

## AIChE Paper on CHEMTRAN

Dr. John Adams presented a paper on November 17 at the Los Angeles AIChE convention entitled "Automation of Group Contribution Techniques For Estimation of Thermophysical Properties". He discussed the computer algorithms which predict properties of mixtures using only two-dimensional chemical structures. These techniques are being applied within CHEMTRAN and have proven to be accurate for these properties. A copy of the paper can be obtained from Dr. John Adams by calling him at (713)627-8945.

## Transport Properties Update

ChemShare has been working on a major update of its pure component data base. As you know this is the largest commercially available database (857 components) and contains all of the data necessary to generate K-values, enthalpies, and densities for process simulation.

This data base is unique in that the data was collected and evaluated by ChemShare. Each datum is traceable to its original source in the literature. In addition, software was developed to perform automatic checks and evaluations of data to rule out inconsistencies occurring in the literature or due to transposition of the data from the literature to the programs.

Now ChemShare has performed a similar task for transport properties and surface tension. We are in the process of adding to the data base the following temperature dependent properties:

1.) Surface Tension
2.) Vapor and liquid viscosity
3.) Vapor and liquid thermal conductivity

Additional mixture correlations for these properties are also being added to DESIGN/2000 so that these properties can be printed in the detailed stream summary. This addition represents about one year's effort in sorting through the literature to find available experimental data. For chemicals where no data exist, predictive techniques have been used.

Of course, it is possible you may have a chemical which isn't in the data base. We are also providing commands to enter any available data you may have. However, if no data is available we have provided a powerful new command to predict data with the STRUCTURE command.

The STRUcture command has been available in ChemTran for a couple of years for prediction of other properties. It allows you to predict thermophysical properties with only a two-dimensional chemical structure. ChemTran takes this input and automatically analyzes it in terms of group-contributions and other characteristics of the chemical structure. This eliminates the need for you to proceed through the time-consuming and error-prone process of applying group contribution techniques by hand.

You will also be able to print out tables, and eventually plots of saturated pure component properties.

Some of the tables are already available in version 9.0. A sample input showing the commands for printing tables of vapor pressure versus temperature and ideal gas heat capacity versus temperature is shown below:

The structure command is for 2,4 dichlorotoluene.

```
*SAMPLE OF PURE COMPONENT DATA GENERATION
COMPONENT=200
STRUCTURE 200=C1-C2,C2=C3,C3-C4,C4=C5,C5-C6,C6=C1,C1-C7,
            C2-CL8,C4-CL9
TAB P-T     200=10,150,5
TAB CP-T    200=10,150,5
RENON K
LATENT HEAT
METRIC UNITS OUT
END
```

The output is shown on the following pages:

```
************  SUMMARY OF SINGLE COMPONENT PROPERTIES  ************

-----------------------------------------------------------------
NONSTANDARD--200            NO.   1            COMPONENT NO. IS  200
-----------------------------------------------------------------
CHEMICAL FORMULA:  C7 CL2 H6
-----------------------------------------------------------------

                              C
                             = -
                        CL -C   C
                            -   =
                            C   C-CH3
                             = -
                              C
                              -
                              CL

-----------------------------------------------------------------
  PROPERTY FOR            VALUE OF                METHOD OF
  GENERAL DATA            PROPERTY              DETERMINATION
--------------------     -----------           --------------------

MOLECULAR WEIGHT          161.031                COMPUTED
NORMAL BOILING POINT     207.39     C           LYD-FOREMAN-THODOS

CRIT TEMPERATURE         441.31     C           LYDERSEN
CRIT PRESSURE            36.639     KG/CM2      LYDERSEN
CRIT VOLUME             0.41200     M3/KGMOL    LYDERSEN
CRIT DENSITY             2.4272     KGMOL/M3    1.0/VC
CRIT COMPRESIBILITY     0.24923                 CALCULATED

DENSITY FACTOR          0.24920                 PC*VC/R*TC
ENTHALPY FACTOR         0.24920                 PC*VC/R*TC
SOLUBILITY PARAMETER     8.4658    (CAL/CM3) 1/2 CALCULATED

VAP PRESS AT TB          1.0332    KG/CM2        DEFAULT
        AT .85*TC        10.045    KG/CM2        DEFAULT
         AT TC           36.639    KG/CM2        DEFAULT

CHAR VOLUME             0.19693E-01M3/KGMOL     V(TB)/(5.7+3*TB/TC)

IDEAL GAS HEAT
   CAPACITY AT 500 K     47.780    KCAL/KGMO/K   BENSON
```

## PARAMETERS FOR TEMPERATURE DEPENDENT EQUATIONS

| PROPERTY | EQUATION | PARAMETERS | UNITS |
|---|---|---|---|
| IDEAL GAS HEAT CAPACITY | T**3 | C1 = -.53790<br>C2 = 0.14144<br>C3 = -.10450E-03<br>C4 = 0.29805E-07 | K, KCAL/KGMO/K |

COMPONENT 200: NONSTANDARD--200

| PT. NO. | TEMP (C) | IDEAL GAS HEAT CAPACITY (KCAL/KGMO/K ) |
|---|---|---|
| 1 | -12.216 | 29.7827 |
| 2 | -9.438 | 30.0404 |
| 3 | -6.660 | 30.2968 |
| 4 | -3.882 | 30.5520 |
| 5 | -1.104 | 30.8059 |
| 6 | 1.673 | 31.0586 |
| 7 | 4.451 | 31.3101 |
| 8 | 7.229 | 31.5603 |
| 9 | 10.007 | 31.8093 |
| 10 | | |
| 11 | | |

COMPONENT 200: NONSTANDARD--200

| PT. NO. | TEMP (C) | VAPOR PRESSURE (KG/CM2 ) |
|---|---|---|
| 1 | -12.216 | 2.045901E-05 |
| 2 | -9.438 | 2.680913E-05 |
| 3 | -6.660 | 3.491121E-05 |
| 4 | -3.882 | 4.518706E-05 |
| 5 | -1.104 | 5.814520E-05 |
| 6 | 1.673 | 7.439498E-05 |
| 7 | 4.451 | 9.466223E-05 |
| 8 | 7.229 | 1.198086E-04 |
| 9 | 10.007 | 1.508499E-04 |
| 10 | 12.784 | 1.889803E-04 |
| 11 | 15.562 | [illegible] |
| 12 | 18.340 | |
| 13 | [illegible] | |

## ChemShare No Longer On UCC in U. S. and Canada

After 10 years of mutual service, ChemShare will no longer be offering our programs on UCC's computers. This is effective December 31, 1982.

Unfortunately the UNIVAC 1108 using EXEC2 is simply too small to be able to handle our programs, even with extended core. For the past 2 years, updating our programs has become very difficult because of the size limitation. Our programs have grown considerably due to our development efforts, and of course with REFINE being incorporated into DESIGN/2000, the problem is about to become worse.

We have sent letters to all our UCC customers during October to tell them of the change, and have been calling each user to get them switched to another service. Any files on account numbers which were assigned by ChemShare on the UCC computer will be deleted as of January 1, 1983. If there are any questions related to this, please call Ken Migas at (713)627-8945.

## New Phone Number For ChemShare's Computers

We have installed a new phone system for our PRIME computer service. This will provide a much stronger signal to your computer terminal, and therefore eliminate a lot of noise on the phone lines coming through our switchboard. The new number is (713)439-0050 and most of our customers are already aware of this. This number is on its own rotary and the computer answers the phone call directly, rather than via the switchboard operator. Questions related to this change can be addressed to Ken Migas at (713)627-8945.

## VESSEL DESIGN Program on ChemShare's Computer

We are pleased to announce that VESSEL, a program for designing and analyzing pressure vessels is now on our PRIME 750. VESSEL is available through a license agreement with Disasu Inc. of Cypress, Texas, the author and developer of the program. VESSEL operates interactively and utilizes keyword, free format techniques. As a result, it is easy to use for data entry and reviewing output.

The ESTIMATE Generation Capabilities may be of particular interest to you. As part of VESSEL's final design, an estimate report is produced. The costs for various material components and labor rates are stored within the program. Specifically, VESSEL can produce a material takeoff report, a labor manhour takeoff report and a total vessel cost report.

If you are interested in more information on VESSEL's capabilities please call Ken Migas at (713)627-8945.

## New Output Option on the PRIME

A new system program called "PRINT" for top of forms control is available for timesharing terminals. This gives you an output file just like a line printer, with each new page starting at the top

"PRINT" is executed at the system level and provides top of forms and page control. The procedure for using PRINT is as follows:

```
OK, PRINT
(PRINT REV. 18.0)
Which file is to be printed?  OUT.TEST
Does the terminal recognize form feeds?  YES
Enter line to start: 1
Enter number of lines to be printed:  99999
Position paper to top of page and press RETURN
```

The file OUT.TEST will be printed with top of forms control in effect.

## Password Control

You can change your password to make use of the protection provided by the PRIME 750. To change your password type the following after login is complete:

```
OK, PASSWD NEW NEW
```

NOTE: When you login the next time the new password will be in effect.

## Using the PRIME for FORTRAN Program Execution

If you have FORTRAN programs which you use frequently, our PRIME 750 can be extremely cost effective and easy to use. A number of our users have compiled FORTRAN programs and execute them with a general reduction in computer costs. Additionally, they are quite satisfied with the turnaround and service which we provide.

We offer free evaluation for program installation on our PRIME system and in most cases, programs can be loaded and operational in just an afternoon.

If you are interested in saving money please give Ken Migas a call at (713)627-8945.

## Prime Configurations

In our last newsletter, we announced that ChemShare has become a Remarketer of Prime hardware. This designation means that ChemShare can sell you a Prime computer with our software, and provide favorable financial terms.

That announcement generated a lot of interest from our customers, and we have learned that there is also a lot of confusion about computers. The biggest confusion is in the basic terms, such as "mini" vs. "micro", and "virtual memory". We would like to clarify these terms as well as describe a new PRIME computer, the small 2250.

A micro computer is essentially the same as what is being called the "Personal Computer". It represents a computer that costs about $5,000 or less. Typically it can have only one person at a time using the machine and has a very small memory, such as 64,000 bytes. The CPU is either an 8 bit or 16 bit machine. It usually has 1 or 2 floppy disk units, a keyboard and a connection to TV screen for input and output. These computers generally use the BASIC language, while some are starting to have limited FORTRAN and PASCAL. These machines are very good for small programs, particularly where they are dedicated to a specific application. Because of the CPU type, some do not have internal checks for errors on the hardware; it is possible that the same problem run twice could give different results.

A mini computer is really only mini in terms of the cost of the machine. Machines made by Prime or Digital Equipment can run as fast as many bigger machines, but they just can't handle as many jobs simultaneously as some of the bigger machines. These mini computers usually cost from $70,000 to $250,000, and can handle a tremendous variety of computations. They typically are 32 bit CPU's with error checking, and have from 512,000 bytes to 2,000,000 bytes of real memory. They usually can handle from 4 to 64 terminals such as CRT display units, have large rigid disk units and a high speed printer. They are supplied with most the common computer languages such as BASIC, FORTRAN, COBOL, and PASCAL. They are as powerful as large scale computers of 5 years ago, but they cost much less. Virtual memory simply is a feature that makes a computer with, for example, 1,000,000 bytes of real memory think it has 4,000,000 bytes of memory. Therefore a small machine can process much more work than was possible before. Also, very large programs such as ChemShare's can run on this type of computer easily and efficiently. Other machines without virtual memory, such as CDC or UNIVAC, require large programs to be broken down into pieces in order to run.

PRIME has just come out with a new computer, labelled the PRIME 2250. This new computer is surprisingly small in size, small in price, and

large in performance.

The machine is compatible with the other PRIME series of computers, so that if you ever outgrow the computer, the next size computer can replace it and all the programs will run on the larger PRIME without reprogramming.

This computer would cost about $60,000 in the U. S., and for this price you would get:

A. 500,000 Bytes of memory (large enough to run ChemShare's programs)

B. 68 Megabytes of disk storage

C. 4 CRT terminals

D. 1 300 line per minute printer

E. 1 console for the computer

F. 1 tape back-up

On this machine, you could easily run our programs, write your own programs and use other software applications such as financial packages.

This new machine runs on the latest version of the operating system called PRIMOS, version 9. We are presently converting our programs to this machine at PRIME's offices in Houston, where a 2250 is available for demonstration.

If you have interest in reviewing this computer call Ken Migas at (713)627-8945.

## PRIME Performance Monitor

ChemShare has developed software for monitoring the performance of any 50 series PRIME computer. This is important in trying to utilize the computer's power to find out areas which are causing any excessive loads, whether in memory, CPU, controllers, etc. In order to evaluate this, we have developed an extensive monitoring program which evaluates all the important computer operations and reports the performance in easy to read graphs. This software is normally sold to people who have their own PRIME computers. If you have interest in this software call Ken Migas at (713)627-8945.

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