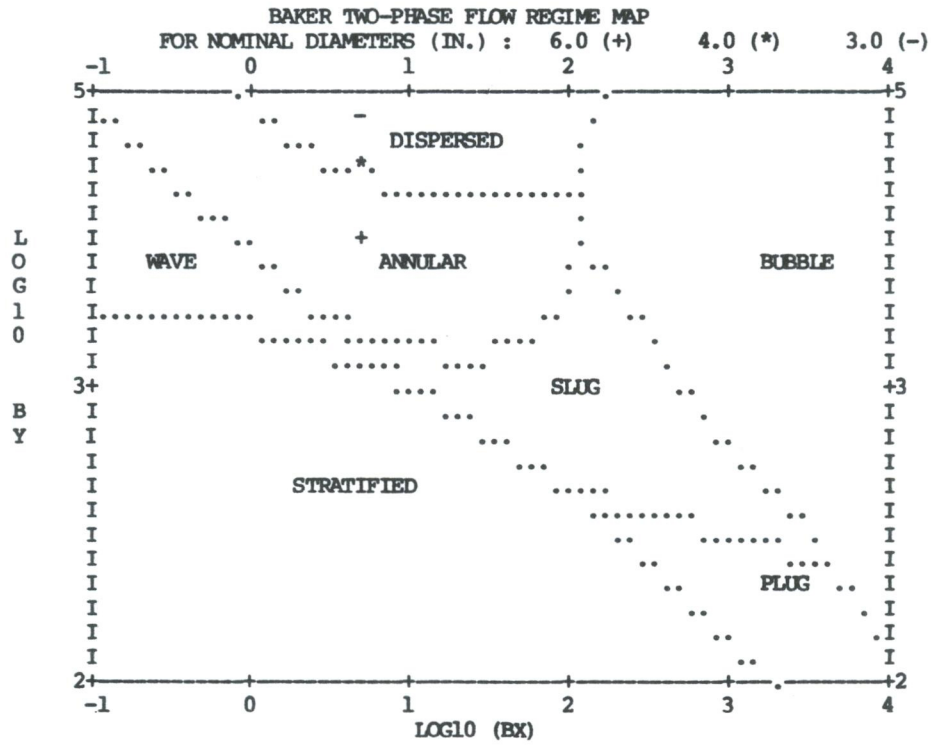
ChemShare

Newsletter No. 202

Month of May, 1982

LINE SIZING



ChemShare

Newsletter No. 202

Month of May, 1982

INDEX

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

Prices

Check out our prices. Why? In March, our competition increased their prices in the U. S. and Canadian markets. We were less expensive before, and now the difference is greater. For those of you who use our competitors, CHECK IT OUT!

Even better, let us check it out for you. Call our sales department TODAY!

ChemShare and PRIME Computers

ChemShare is pleased to announce that we have signed an agreement with Prime Computers to jointly market Prime Computers with ChemShare's software. What this means is that ChemShare can sell you a Prime computer at a reduced price for the hardware and you can have ChemShare's software on that computer with whatever financial arrangement best meets your needs. The reason we have decided to make this arrangement is that we firmly believe that as computers become smaller, faster, and cheaper, developers of software must be more involved with integrating hardware and software. Graphics, data base management systems, and personal computers are changing the hardware capabilities available to the software developer. Without a closer association with hardware our perspective on product development would be limited. We believe that as a user of our software, you will gain by this association.

One of the gains, as we mentioned, can be less expensive hardware. Without going into a lot of details, you can now get computers that sit in a corner of a room, with 4 terminals and a high speed printer for less than $3,500.00 per month in the U. S. including maintenance. To operate one is simple and almost anyone can do it. (Prices outside the U. S. are typically higher).

Over the last year, we know of 4 PRIME computers sold in the Houston area to relatively small companies. All of them have ChemShare's software loaded. Each has recovered costs by not spending money at outside service bureaus. None of them has had any difficulties in learning how to run the computer.

We plan to bring to you typical PRIME systems and give you some idea on prices. If you have any interest in exploring computers with us, call (713)627-8945. Ask for your account representative.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

REFINE Manuals

This is the last word on the new REFINE manuals!

THEY ARE DONE!!

By the time you are reading this newsletter distribution has already begun. Remember, now ChemShare has the only current documentation.

REFINE Into DESIGN/2000

We are currently proceeding with the integration of REFINE crude units into DESIGN/2000. Although this project is only in the initial stages, the progress has been very good. When this work is finished, you will be able to simulate flow sheets in DESIGN/2000 containing REFINE crude units with the same ease as regular distillation columns. It is too early to specify a precise completion date, but we plan to have this project finished this year.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

Viscosity Specification

For refiners making lubricating oils, typical specifications available in simulation programs have not adequately met their needs. In particular, a direct viscosity specification on the products has not been provided.

Now in REFINE versions 8.4067 (08 MAR 82) and later, you can enter a viscosity specification on a product and converge rigorously to that value. In order to do this, you must enter viscosity data for each feed. The viscosity specification is allowed on one product.

The command is:

PROduct SPEcification = value, VIScosity SET X, product specified, product varied

PRO SPE = 1.6, VIS SET 1, 5, 6

This command will set the viscosity of product 5 at 1.6, at the temperature for set 1, by varying the rate of product 6.

Again, ChemShare has the only software offering this important feature.

New Molecular Weight Option

The API has come out with a new equation for calculating molecular weights of petroleum fractions. This technique primarily affects the higher boiling fractions. We have added this option to REFINE on versions 8.4067 (08 MAR 82) and later. The command for this new option is:

DATa MOLecular KEY = 3

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

Announcing Line Sizing in DESIGN/2000

The first of our sizing options is about ready for release. A copy of the line sizing output form DESIGN/2000 is shown below for your review and comments.

Sizing can be performed for both single and two phase lines; vertical, horizontal or inclined. The sizing criterion can be either allowable pressure drop or maximum velocity. Alternatively the user may specify a particular pipe size to calculate pressure drop and velocity.

You will notice that we present to you three pipe sizes: target, larger and smaller, and print such details as Reynolds number and friction factor under each pipe size. The two phase methods used are those of Lockhart-Martinelli for horizontal lines and Orkiszewski for vertical lines. For two phase lines on the Baker flow regime map is also presented so that you can easily see how close you are to a potential flow regime boundary.

Documentation and release dates will be provided in the next newsletter. This option is running on our PRIME computers, if anyone needs to use it now.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

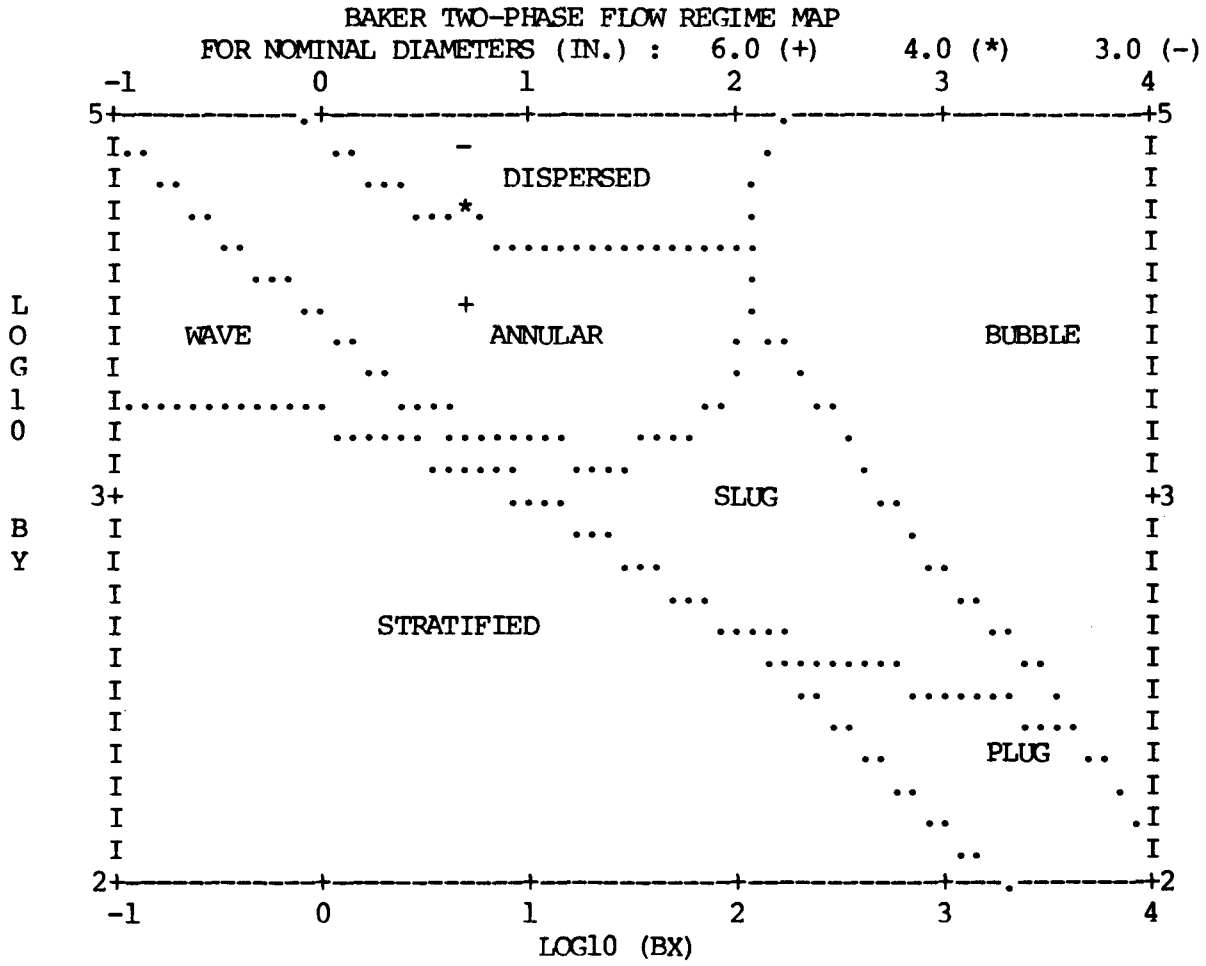
PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

```
* SAMPLE FOR LINE SIZING USING MODIFIED EXPANDER PLANT
HEAT EXCH7=H137,21,-16, DEL=10
TEMP OUT=-45
FLASH DRUM19=S306,16,-11,-44
EXPANDER37=E33,11,-31,-33
PRESS OUT=300



GENERAL
COMPONENTS=2,3,4
FLOW21=1100,100,100
TP21=100,800
KVAL
SIZE LINES
   USE STREAMS = 16, 11, 33
   DIRECTION OF FLOW = HORI,HORI,HORI
   MAXIMUM DELTAP PER HUNDRED FEET = 6.0, 1.0, 0.9
END

********** LINE SIZING RESULTS FOR 2 PHASE STREAM 16 **********

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

		LARGER	TARGET	SMALLER
I.D. FOR BAKER MAP		+	*	-
NOMINAL DIAMETER	IN.	6.000	4.000	3.000
INTERNAL DIAMETER	IN.	6.065	4.026	3.068
DELTA P (FRICTION)	PSIA	0.1824	1.865	7.583
DELTA P (ELEVATION)	PSIA	0.0000	0.0000	0.0000
DELTA P (TOTAL)	PSIA	0.1824	1.865	7.583
MEETS DELTA P SPEC		YES	YES	NO
OUTLET PRESSURE	PSIA	789.8	788.1	782.4
LIQUID VELOCITY	FT/SEC	0.3764	0.8542	1.471
VAPOR VELOCITY	FT/SEC	5.482	12.44	21.42
2-PHASE VELOCITY	FT/SEC	4.281	10.34	19.01
REYNOLDS NUMBER		0.1724E 07	0.2597E 07	0.3407E 07
REYNOLDS NUMBER		0.1186E 06	0.1787E 06	0.2345E 06
FROUDE NUMBER		1.277	11.29	102.6
FLOW REGIME		ANNULAR	DISPERSED	DISPERSED
FRICTION FACTOR		0.1534E-01	0.1651E-01	0.1745E-01
FRICTION FACTOR		0.1896E-01	0.1876E-01	0.1901E-01
2-PHASE DENSITY	LB/FT3	8.106	7.615	7.132
LIQUID HOLDUP		0.1759	0.1508	0.1261

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793



THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

UNIQUE CHEMSHARE FEATURES APPLICABLE TO GAS PROCESSING

Some people ask us how our software compares with others. In order to answer that question, we compiled the features that are unique just for gas processors.

- CO_2 solids prediction
- AMINE treating - (MEA/DEA)
- SELEXOL Solvent thermodynamics
- APISOAVE Thermodynamics for natural gas with H_2S, CO_2, N_2, CO
- Plotted outputs of:
  - Heat exchangers
  - Phase Envelope
  - Shortcut column
  - Column traffic
  - Composition profiles
- Ratio of heat capacities, C_p/C_v, reported for compressor module
- Heat capacity of each stream calculated
- 1981 National Bureau of Standards transport properties technique for viscosity and thermal conductivity
- Heating value of streams
- Critical temperatures and pressures of streams calculated rigorously
- Reid vapor pressure
- Line sizing for streams
- Equilibrium reactor modules for syngas
- Faster convergence techniques on distillation columns

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

SELEXOL® Solvent Update

The advertisement shown on the following page has been published in the Oil and Gas Journal, Hydrocarbon Processing, and Chemical Engineering Progress. As expected, there have been a large number of responses from all over the world. Many companies have contacted Allied Corporation for the paperwork required to get their passwords. Usage has shown that by integrating the SELEXOL thermodynamics into DESIGN/2000 it is extremely easy to model complete plants. Convergence on the distillation columns and recycles is fast and easy. Remember, any questions on this option should be directed to Dr. John Adams at (713)627-8945.

As of April 1, 1982, Norton Company has purchased the Selexol Solvent organization from Allied Corporation. The Selexol Solvent group is at the same location in New Jersey, but is now a part of the Norton Company.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

Fast, rigorous simulation solves processing problems.

New, faster way to look at SELEXOL® options

*ChemShare announces the first complete, rigorous computer simulation of SELEXOL® solvent gas purification units.**

In just a few hours, you can set up a computer model of an entire SELEXOL solvent acid-gas-removal unit, then use it to:

1. evaluate various equipment configurations and size the equipment;
2. determine optimum circulation rates and cooling rates; and,
3. study your unit's ability to handle different feed streams.

You can do all of this for any type of SELEXOL solvent plant—CO_2 removal, ammonia synthesis gas purification, sulfur removal, coal gasification, and others.

Allied's SELEXOL solvent data assures accuracy.

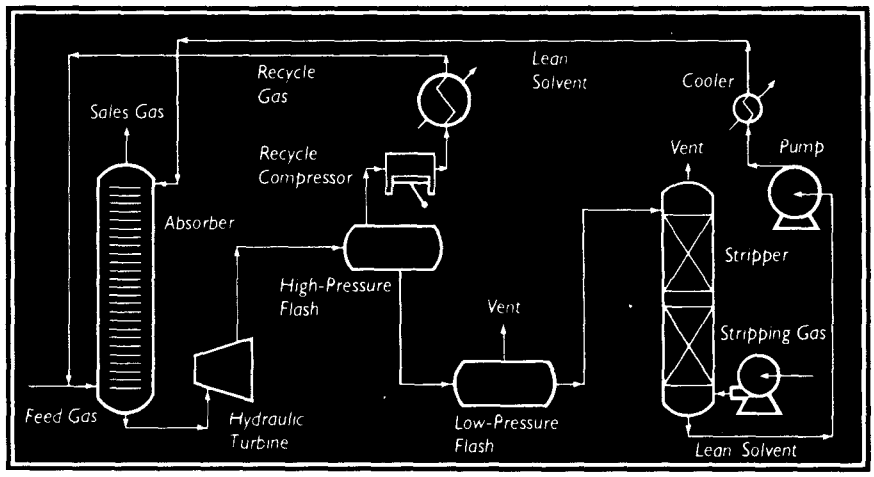
Allied Corporation has provided proprietary vapor-liquid-equilibrium and enthalpy data, which has been added to the DESIGN/2000SM data bank. This laboratory data, combined with ChemShare's rigorous process calculations, gives you the accurate results you need for design and operating decisions.

Rigorous simulation of the entire unit

ChemShare's DESIGN/2000 process simulation program duplicates all of the equipment in a SELEXOL unit: absorber column, flashes, compressors, pumps, heat exchangers and stripper column. Using simple, English-language commands, you specify each piece of equipment and its place in the flowsheet. Then, specify the feed gas, and DESIGN/2000 calculates not only the sales gas product, but all intermediate streams, including gas and solvent recycles. Or, since DESIGN/2000 solves for the unknown, you can specify the gas product and let DESIGN/2000 calculate equipment parameters.

*Because SELEXOL solvent unit simulations involve proprietary and confidential information, a secrecy agreement with Allied Corporation is required before simulation results can be released.

®SELEXOL is a registered trademark of Allied Corporation.



You can simulate this entire flowsheet in a single computer run. Allied's proprietary SELEXOL solvent lab data assures accurate results.

For each simulation, you get a detailed printout with all the information you need for your evaluation, including:

- feed analysis
- absorber flowrates, tray-by-tray
- absorber profiles, tray-by-tray
- finished product analysis
- absorber bottom product analysis
- tray-by-tray composition
- graph of separation parameters vs. temperature
- stream summaries
- equipment summaries

*Get a copy of this simulation.**

Call us, or write to us on your letterhead, and we'll send you a brochure explaining the SELEXOL solvent process, plus an eight-page brochure that will give you a clear idea of how ChemShare works. If your company is a SELEXOL solvent licensee, we can provide the input and printout for a complete simulation. We can also arrange a no-obligation, hands-on demonstration for you.

Four important things you should know about ChemShare.

1. Our programs work. Process calculations are rigorous and accurate.
2. The programs are easy to use, without special training in computers or computer languages.
3. You don't have to own a computer.
4. The costs are nominal.

ChemShare®

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

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

ChemShare

Newsletter No. 202

Month of May, 1982

REID Vapor Pressure in DESIGN/2000

ChemShare can calculate the Reid vapor pressure in accordance with ASTM D323-79. You can add a command in the GENERAL section to calculate the REID VAPOR PRESSURE on any stream in your flowsheet.

The command is:

REID vapor pressure = (stream numbers), for example,

REID = 5, 10, 30

The calculated vapor pressure is printed in the detailed stream output.

This command is available on DESIGN/2000 version 8.4067 (08 MAR 82) or later.

Additional Specification Units For DESIGN/2000

BARRELS, GALLONS, POUNDS!

A new capability on the rigorous distillation unit in DESIGN/2000 has been added to allow you to specify product rates in units other than moles. You can set barrels, gallons, pounds, or other units. This is done using these new commands:

TOTal PROduct TOP (Q units/ t units) =
TOTal PROduct SIDe n (Q units/ t units) =
TOTal PROduct BOTtom (Q units/ t units) =

The PRODUCT command must still be entered and is used as a guess for the molar equivalent of the specifications. This command is available on DESIGN/2000 versions 8.4067 (08 MAR 82) and later.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

SOUR WATER UPDATE!

NH_3, H_2O, H_2S, CO_2

The APISOUR correlation, which is based on API Report No. 955, has been expanded to allow use of organic acids and caustics. The following acids are allowed:

Name	Component No.
Formic Acid	3038
Acetic Acid	1001
Propionic Acid	2040
Butryic Acid	2041

The allowed caustics are sodium hydroxide or potassium hydroxide. These components have been assigned the following component numbers.

Name	Component No.
NaOH (Sodium hydroxide)	9003
KOH (Potassium hydroxide)	9004

Either acid or caustic can be entered directly on a column tray to change the pH, and therefore, the solubilities of NH3, CO2, and H2S in water. These options will be available in DESIGN/2000 versions 8.4067 (08 MAR 82) and later.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982

CHEMTRAN

For those of you not familiar with CHEMTRAN, we felt an overview of this program's capabilities and applications would be of general interest.

CHEMTRAN is a separate program from DESIGN/2000 and REFINE. It is normally used to pass information to DESIGN/2000, where heat and material balance simulations are done. CHEMTRAN is used to generate pure component information and/or fit some form of mixture data to help generate K-values, enthalpies, and densities that are to be used in a simulation in DESIGN/2000.

CHEMTRAN has 2 major divisions:
1) Pure component physical properties
2) Mixture properties

1. Pure Component Physical Properties

The pure component section of CHEMTRAN is typically used to generate pure component properties for components which are not in the ChemShare pure component data base. At present, this data base contains 857 components, making it the largest data base commercially available. Data for this data base has been collected and correlated by ChemShare. It has been checked and cross checked for accuracy and each item in the data base can be traced back to the primary literature sources.

As there are thousands of components which are not in the data base due to limited published information for their physical properties, it is necessary to estimate their properties. These properties are critical temperature, pressure, volume, solubility factor, acentric factor, molecular weight, boiling point, ideal gas heat capacities, density, latent heat, and vapor pressure. ChemShare has created a physical properties generator which is unique in a couple of ways. It is the only one commercially available, and it is easy to use.

It works by simply describing the molecular structure of the component to CHEMTRAN.

Let's take 2,4- dichlorotoluene as an example for generating physical properties.

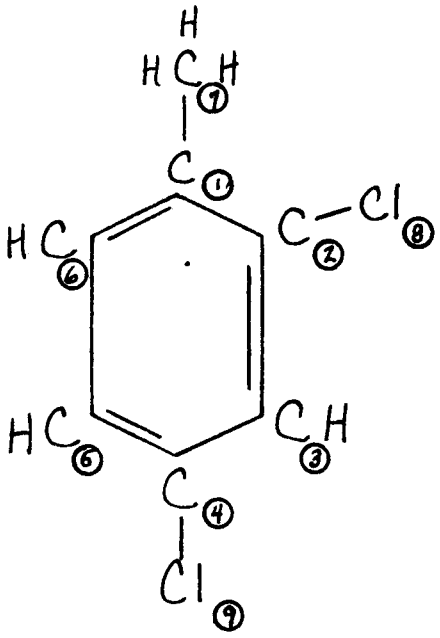
THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

ChemShare

Newsletter No. 202

Month of May, 1982



There are various techniques available in the literature for generating physical properties, such as Benson, Parr, and Lyderson. Each of these methods requires a different description of the same bond structure. Some structures are difficult to describe and doing these calculations by hand may require a full day. In CHEMTRAN a single unified input structure is used for generating all the properties. For example, the component previously described would be entered into CHEMTRAN by numbering all the non-hydrogen atoms and then describing the bond connections to CHEMTRAN once. Example:

```
*SAMPLE OF PURE COMPONENT DATA GENERATION
COM=200
STRUCTURE 200=C1-C2,C2=C3,C3-C4,C4=C5,C5-C6,C6=C1,C1-C7,
          C2-CL8,C4-CL9
END
```

This unified input structure looks simple, and it is. As far as we know, ChemShare is the only company who has been able to set up a unified method for predicting pure component properties. Although approaches to this have appeared they have not been nearly as complete in predicting all the properties of pure components needed for heat and material balance calculations. The output follows on the next page.

The input coding is in your present CHEMTRAN manual, but questions can be addressed to Dr. John Adams or Customer Support at (713)627-8945.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

**********SUMMARY OF MESSAGES FOR IDL GAS HEAT CAP ESTIMATION**********

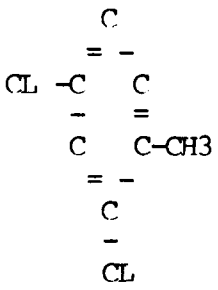
FOR COMPONENT 200:
BENSON'S GROUP (C) - (CB) (H) (H) (H)
HAS 2 SUBSTITUTIONS : (C) - (C) (H) (H) (H)

1CHEMSHARE CHEMTRAN VERSION 8.3268(02MAR82) 19MAR82 13:37:30
0SAMPLE OF PURE COMPONENT DATA GENERATION PAGE 2

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

NONSTANDARD--200 NO. 1 COMPONENT NO. IS 200

CHEMICAL FORMULA: C7 CL2 H6



PROPERTY FOR GENERAL DATA	VALUE OF PROPERTY		METHOD OF DETERMINATION
MOLECULAR WEIGHT	161.031		COMPUTED
NORMAL BOILING POINT	405.29	F	LYD-FOREMAN-THODOS
CRIT TEMPERATURE	826.34	F	LYDERSEN
CRIT PRESSURE	521.12	PSIA	LYDERSEN
CRIT VOLUME	6.5996	FT3/LBMOL	LYDERSEN
CRIT DENSITY	0.15152	LBMOL/FT3	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
CHAR VOLUME	0.31546	FT3/LBMOL	V(TB)/(5.7+3*TB/TC)
IDEAL GAS HEAT CAPACITY AT 500 K	47.780	BTU/LBMO/R	BENSON

ChemShare

Newsletter No. 202

Month of May, 1982

Mixture Properties

By mixture properties we are referring to the properties needed to perform heat and material balances such as K-values and enthalpies. After these calculations are performed other properties are also needed. Densities are required to convert from molar flow units to volume flow units. Transport properties are needed for line and equipment sizing.

DESIGN/2000 contains many correlations to estimate all the properties needed for most flowsheet simulations -- 21 K-value correlations, 17 enthalpy correlations, 9 density correlations, and 3 transport property correlations. This is the largest number of options commercially available. There are systems where their accuracy may not be sufficient. For example, K-values for the acetone-water system can be predicted by UNIFAC and depending on your needs these predictions may work very well. However, since UNIFAC is designed to be a general correlation for chemical systems it cannot provide the accuracy obtained by fitting vapor-liquid equilibrium data. Similar statements can be made for other correlations. For example, although equations of state work very well for light hydrocarbons their accuracy can deteriorate for heavier hydrocarbons and inorganic gases such as CO2, H2S, etc. In the case of the APISOAVE correlation some of this data fitting has been done and the resulting parameters are stored in DESIGN/2000. However, it is possible that data for additional chemicals may be needed to supplement the basic correlation.

When we discuss K-value data, we are referring to laboratory vapor-liquid compositions at various temperatures and pressures. There is a tremendous amount of this data which has been published. Our customer support service has ready access to much of this data and can help determine if it is available for a specific system.

Your company may also have, or wish to measure, its own data for a particular system. The latter step may be useful when data is missing for an important composition or temperature region. In some systems, heats of mixing data are also needed to represent accurately heat changes in a flowsheet. This data is also available in the literature.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

The published data can be a table or graph of various temperatures and pressures where the composition of the liquid and the composition of the vapor are reported. This data would be entered with a T-P-Y-X command. There are several other ways data could be reported. CHEMTRAN has 13 different options for entering this data. These options cover just about all the usual ways data is found in the literature.

The following is an example for an acetone-water system with the required CHEMTRAN input:

```
*ACETONE WATER DATA FIT
COMP=1002,62
T-X(C,MMHG) 1002,62=760,100,0,89.6,.015,79.4,.036,68.3,.074,63.7,.175,
            61.1,.259,60.5,.377,59.9,.505,59,.671,58.1,.804,57.4,.899,
            74,.05,68.9,.082,65.8,.125,62.9,.220,62.7,.445,58.3,.66,57.8,.76,
            57.3,.865,56.7,.93,83,.023,76.5,.041,66.2,.12,61.8,.264,61.1,.3,
            60,.444,59.7,.506,59.5,.538,58.9,.609,58.5,.661,57.4,.793,57.1,.85
WILSONK
YEN ALEXANDER H
FILE NEW=ACET,DATA,H20
END
BOTTOM
```

Any VLE data you enter can be curve fitted to one of 6 equation options- Wilson, Renon (NRTL), UNIQUAC, Peng-Robinson, Soave, and APISOAVE. The results of this data reduction are a set of binary interaction coefficients which can be stored in a special file for DESIGN/2000. The command for creating this file is:

FILE NEW = nam1, nam2, nam3

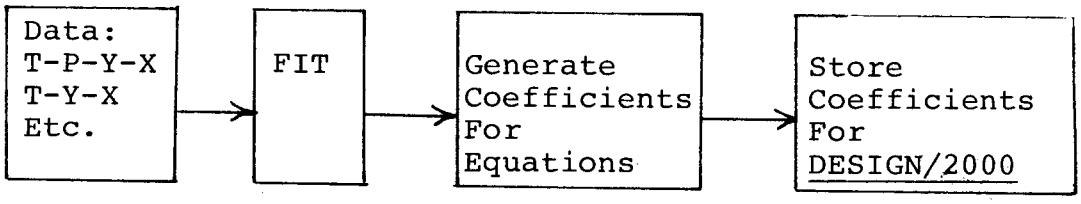
An objective function is also necessary for the data reduction. The program minimizes the error in this function. The default function is normally K-values (OBJFUN=3). However, other options are available. Various error reports are printed to let you examine how well the curve fit matches your data. Graphs are also presented to provide at a glance the results of the data reduction.

Once the coefficients for the equation have been generated, they can be used in DESIGN/2000 to calculate K-values at any temperature and pressure by entering the file name into DESIGN/2000 with the CHE FIL= command in the GENeral section.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

The overview of this data reduction is:



Some output for the acetone-water data fit is shown below:

```
****** REDUCTION OF VAPOR LIQUID EQUILIBRIUM DATA FOR SYSTEM  1 ****
EQUATION OPTION IS WILSON
DATA TYPE IS TX
NUMBER OF ITERATIONS=    9
SUM OF SQUARES OF THE OBJECTIVE FUNCTION=  0.2109462E-01
STANDARD ERROR OF ESTIMATE=  0.1844548E-01
      COMPONENTS IN SYSTEM
```

NO.	CODE NO.	NAME
1	1002	ACETONE
2	62	WATER

V-L-E DATA

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMPOSITION (MOLE FRACTION) COMP	VAP-CAL'D	LIQUID	VALUE OF OBJECT FUNCTION
1	211.988	14.6961	1002	0.000000	0.000000	-0.00035
1			62	1.000000	1.000000	
2	193.268	14.6961	1002	0.371538	0.015000	-0.06883
2			62	0.628462	0.985000	
3	174.908	14.6961	1002	0.576963	0.036000	-0.04381
3			62	0.423037	0.964000	
4	154.928	14.6961	1002	0.713276	0.074000	0.05954
4			62	0.286723	0.926000	
5	146.648	14.6961	1002	0.786160	0.175000	0.00951
5			62	0.213840	0.825000	
6	141.968	14.6961	1002	0.808290	0.259000	0.03881
6			62	0.191710	0.741000	
7	140.888	14.6961	1002	0.822784	0.377000	0.01601
7			62	0.177216	0.623000	
8	139.808	14.6961	1002	0.837099	0.505000	0.00050
8			62	0.162901	0.495000	
9	138.188	14.6961	1002	0.861385	0.671000	-0.01411
9			62	0.138615	0.329000	
10	136.568	14.6961	1002	0.892930	0.804000	-0.02097
10			62	0.107070	0.196000	

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793

TABULATED ACTIVITY COEFFICIENT AT CONSTANT PRESSURE

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMP	CALC	EXPER	PERCENT RELATIVE ERROR
1	211.988	14.6961	1002	N/A	N/A	N/A
1			62	1.000000	0.000000	0.00000
2	193.268	14.6961	1002	9.821602	9.365011	4.87549
2			62	1.001353	0.943684	6.11098
3	174.908	14.6961	1002	8.199156	8.016010	2.28475
3			62	1.007160	0.971864	3.63184
4	154.928	14.6961	1002	6.164395	6.700273	-7.99784
4			62	1.026400	1.099258	-6.62798
5	146.648	14.6961	1002	3.493340	3.608214	-3.18370
5			62	1.112427	1.131045	-1.64610
6	141.968	14.6961	1002	2.559608	2.725929	-6.10144
6			62	1.214367	1.272306	-4.55384
7	140.888	14.6961	1002	1.868404	1.944009	-3.88914
7			62	1.405628	1.438452	-2.28184
8	139.808	14.6961	1002	1.469848	1.505864	-2.39176
8			62	1.698906	1.711460	-0.73356
9	138.188	14.6961	1002	1.189445	1.201335	-0.98971
9			62	2.302412	2.285642	0.73371
10	136.568	14.6961	1002	1.067173	1.070845	-0.34290
10			62	3.136592	3.092196	1.43574
11	135.308	14.6961	1002	1.018523	1.021050	-0.24742
11			62	4.118987	4.055183	1.57339

TABULATED FUGACITIES BASED ON EXPERIMENTAL DATA

PT. NO.	TEMP (F)	PRESSURE (PSIA)	COMP	FSS	PHI	LN(ACT)
1	211.988	14.6961	1002	N/A	0.985469	N/A
1			62	14.494196	0.992934	0.00000
2	193.268	14.6961	1002	38.189705	0.982518	2.23698
2			62	9.864405	0.992778	-0.05796
3	174.908	14.6961	1002	28.806126	0.980381	2.08144
3			62	6.588386	0.992843	-0.02854
4	154.928	14.6961	1002	20.681587	0.978245	1.90215
4			62	4.109994	0.992856	0.09464
5	146.648	14.6961	1002	17.881596	0.977289	1.28321
5			62	3.344395	0.993024	0.12314
6	141.968	14.6961	1002	16.434254	0.976775	1.00281
6			62	2.967551	0.993027	0.24083
7	140.888	14.6961	1002	16.113270	0.976641	0.66475
7			62	2.886115	0.993098	0.36357
8	139.808	14.6961	1002	15.797079	0.976506	0.40937
8			62	2.806584	0.993170	0.53735
9	138.188	14.6961	1002	15.331970	0.976303	0.18343
9			62	2.690859	0.993304	0.82665
10	136.568	14.6961	1002	14.877535	0.976098	0.06845
10			62	2.579346	0.993492	1.12888
11	135.308	14.6961	1002	14.531330	0.975937	0.02083
11			62	2.495597	0.993732	1.40000
12	165.188	14.6961	1002	24.600071	0.979348	2.02472

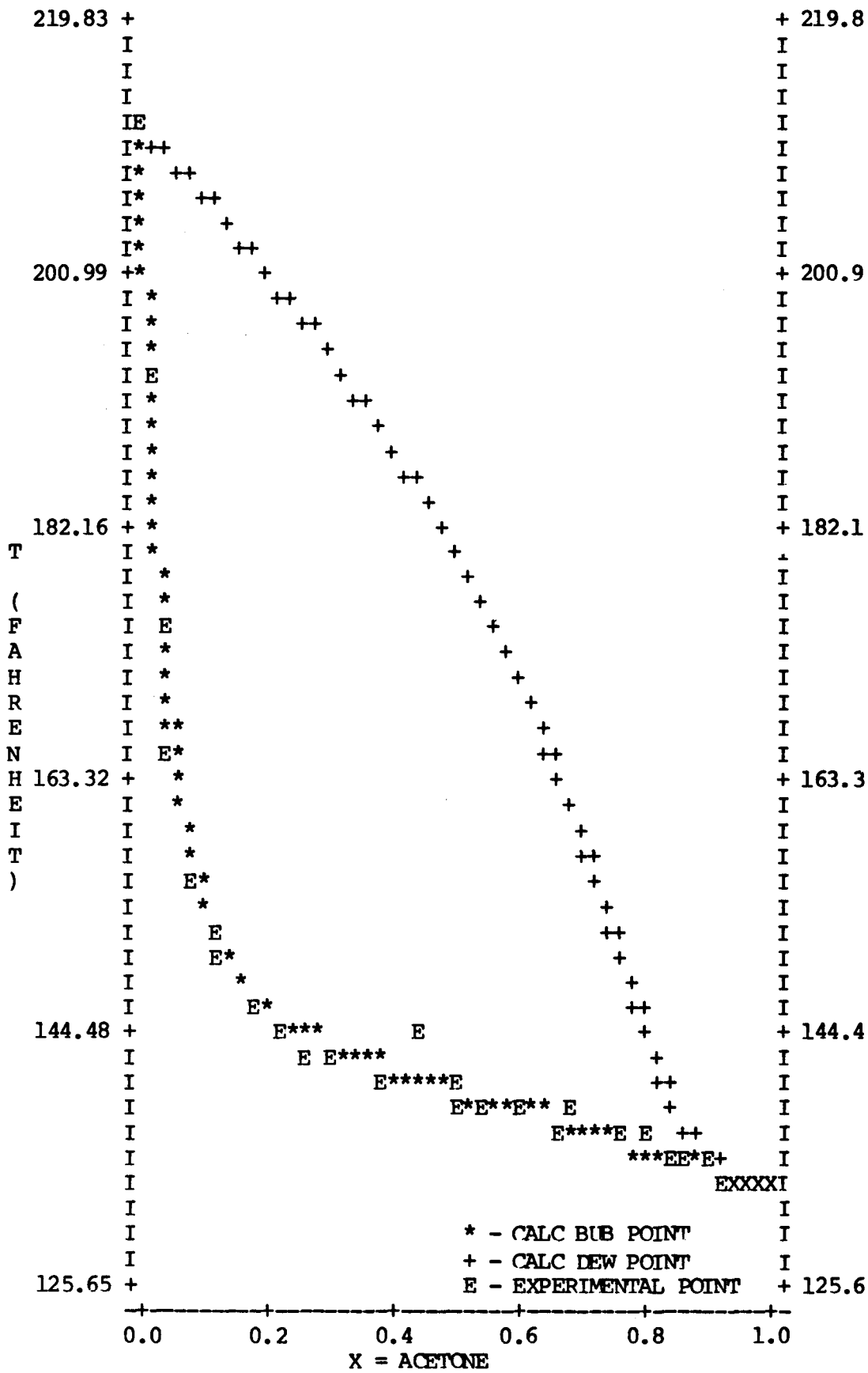
BUBBLE POINT TEMPERATURES

PT. NO.	PRES (PSIA)	(FAHRENHEIT) DATA	CALCULATED	PERCENT DIFFERENCE
1	14.696	211.988	211.959	-1.36E-02
2	14.696	193.268	189.574	-1.91E 00
3	14.696	174.908	172.463	-1.40E 00
4	14.696	154.928	158.386	2.23E 00
5	14.696	146.648	147.177	3.61E-01
6	14.696	141.968	144.128	1.52E 00
7	14.696	140.888	141.760	6.19E-01
8	14.696	139.808	139.835	1.92E-02
9	14.696	138.188	137.444	-5.38E-01
10	14.696	136.568	135.470	-8.04E-01
11	14.696	135.308	134.146	-8.58E-01
12	14.696	165.188	165.711	3.17E-01
13	14.696	156.008	156.673	4.26E-01
14	14.696	150.428	150.712	1.89E-01
15	14.696	145.208	145.288	5.54E-02
16	14.696	144.848	140.707	-2.86E 00
17	14.696	136.928	137.606	4.95E-01
18	14.696	136.028	136.124	7.03E-02
19	14.696	135.128	134.595	-3.95E-01
20	14.696	134.048	133.784	-1.97E-01
21	14.696	181.388	181.679	1.61E-01
22	14.696	169.688	169.755	3.98E-02
23	14.696	151.148	151.212	4.25E-02
24	14.696	143.228	144.000	5.39E-01
25	14.696	141.968	143.173	8.49E-01
26	14.696	139.988	140.721	5.24E-01
27	14.696	139.448	139.820	2.67E-01
28	14.696	139.088	139.363	1.98E-01
29	14.696	138.008	138.347	2.45E-01
30	14.696	137.288	137.591	2.21E-01
31	14.696	135.308	135.632	2.40E-01
32	14.696	134.768	134.804	2.67E-02

BUBBLE POINT PRESSURES

PT. NO.	TEMP (F)	(PSIA) DATA	CALCULATED	PER CENT DIFFERENCE
1	211.988	14.6961	14.7161	1.36E-01
2	193.268	14.6961	15.7215	6.98E 00
3	174.908	14.6961	15.3511	4.46E 00
4	154.928	14.6961	13.8043	-6.07E 00
5	146.648	14.6961	14.5531	-9.73E-01
6	141.968	14.6961	14.1129	-3.97E 00
7	140.888	14.6961	14.4554	-1.64E 00
8	139.808	14.6961	14.6885	-5.17E-02
9	138.188	14.6961	14.9087	1.45E 00
10	136.568	14.6961	15.0123	2.15E 00
11	135.308	14.6961	15.0301	2.27E 00
12	165.188	14.6961	14.5589	-9.33E-01
13	156.008	14.6961	14.5206	-1.19E 00
14	150.428	14.6961	14.6200	-5.18E-01
15	145.208	14.6961	14.6742	-1.49E-01
16	144.848	14.6961	15.8919	8.14E 00
17	136.928	14.6961	14.5045	-1.30E 00
18	136.028	14.6961	14.6688	-1.86E-01
19	135.128	14.6961	14.8488	1.04E 00
20	134.048	14.6961	14.7712	5.11E-01
21	181.388	14.6961	14.6189	-5.25E-01
22	169.688	14.6961	14.6784	-1.21E-01
23	151.148	14.6961	14.6789	-1.17E-01

T VS. X FOR: ACETONE - WATER AT P = 14.69 PSIA



The graphical output quickly shows you how good the fit is in relation to experimental data. The "E"s on the graph above are the experimental data points. From this plot, it appears to be a reasonably good fit.

The tabulated data presents actual deviations for each data point. The output gives you the following major reports:

1. V-L-E Data comparison at each point
2. Activity coefficients at constant pressure
3. Fugacities
4. Bubble point temperatures comparison
5. Bubble point pressures comparison

The acetone-water mixture is a binary mixture which can easily be handled by CHEMTRAN. There are also many multi-component mixtures where the data may be available in a ternary or quaternary form. CHEMTRAN is the only commercially available program that will accept data of any form directly and reduce it.

Previously mentioned was a thermodynamic correlation called UNIFAC. Where UNIFAC can be used, experimental data is not always needed, but if the data is available it is best to use it. However, in a situation where a quick calculation needs to be made, or the data is not readily available, UNIFAC can be used to generate K-values for many multi-component systems. It can also be used to generate coefficents for specific binary pairs. This is a useful option for multi-component mixtures where there is no data for some of the components.

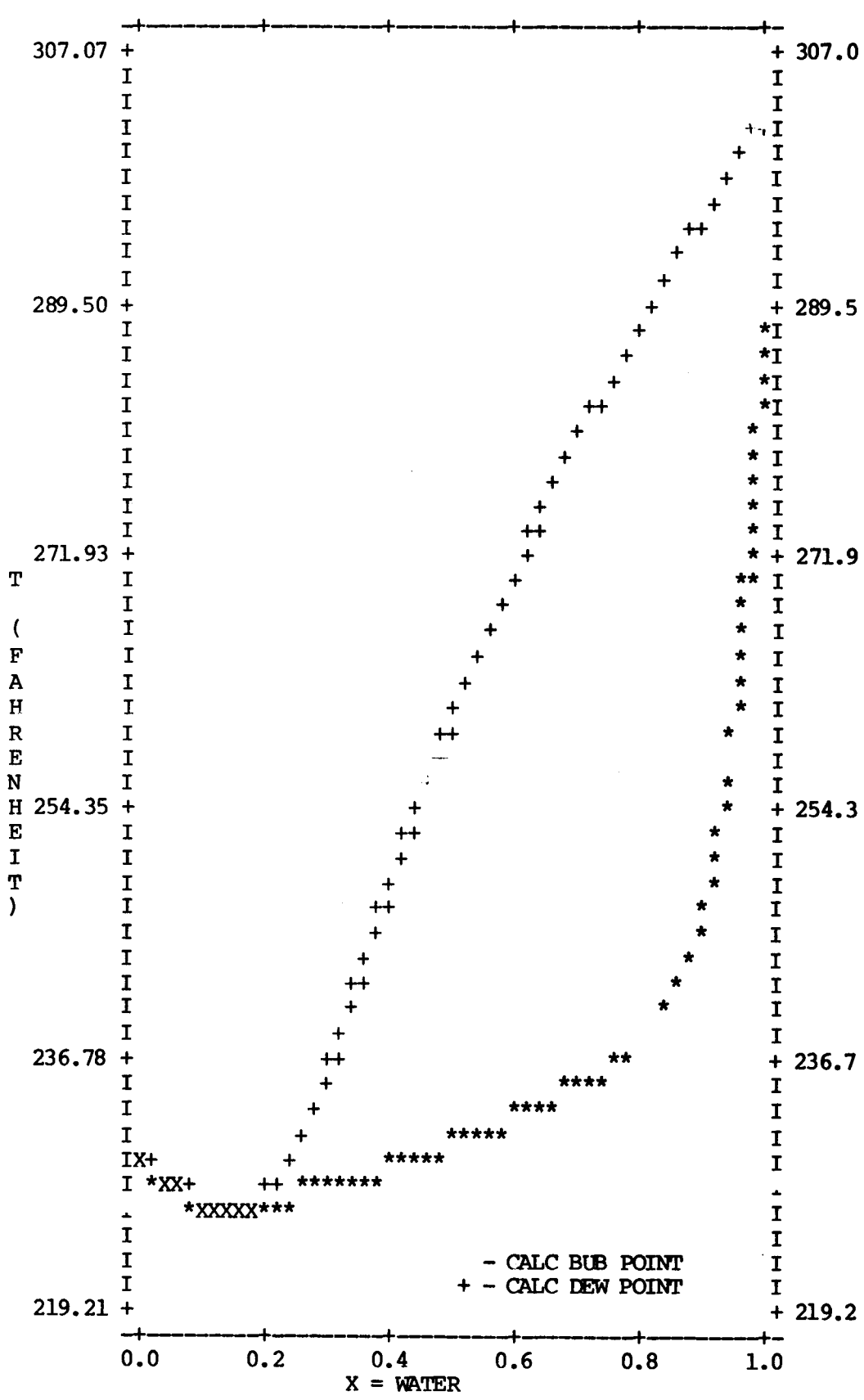
Another useful feature of CHEMTRAN combines the VLE graphics capabilities with the group contribution techniques, in particular, UNIFAC. This combination allows you to examine the VLE behavior of binary systems and determine azeotropes from the structures of chemicals. If the chemicals are in the data base, structures are stored in the program and do not have to be entered. By simply running the following input for the mixture of acetone and water, we can plot the azeotrope. The input is simply:

```
*AZEOTROPE PLOT FOR ACETONE AND WATER
COM=62,1002
UNIFACK
GRA T-X 62,1002=70
END
```

The graphical output is shown on the next page.

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

PHONE: 713-627-8945 HOTLINE: 713-627-1760 TWX: 910-881-2793



This application can be extended to chemicals where no data is available. Since UNIFAC is a group contribution technique, the unified structure command can be used. Then it is possible to generate pure component properties and VLE graphs with a few simple structure commands.

The CHEMTRAN manual also covers all mixture input commands. Any questions or ideas for CHEMTRAN should be directed to Dr. John Adams or Customer Support.