ChemShare

Newsletter No. 104

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THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

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

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MAJOR ENHANCEMENTS!!

		Version Dates
1.	Unlimited size flowsheets in DESIGN/2000	01 Jul 80
2.	Amine treating in DESIGN/2000	01 Jul 80
3.	Three phase distillation in DESIGN/200	by request
4.	Three phase flash in DESIGN/2000	by request
5.	APISOAVE thermodynamic correlation in DESIGN/2000	01 May 81
6.	CO2 freeze prediction in DESIGN/2000	01 Jul 81
7.	Ratio of heat capacities in DESIGN/2000	01 Apr 81
8.	Braun K-10 thermodynamic option in REFINE	01 Jun 81
9.	New thermal conductivities in REFINE	01 Jan 81
10.	Plotting of data fits in CHEMTRAN	01 Jan 81

ChemShare is pleased to announce the above new capabilities to our software. Our continued development efforts provide you with the most current technology today. This newsletter will give you overviews of each of the above items. Detailed documentation will be forthcoming. If there is need to run any of these items immediately, call the Hotline (712-627-8945), for detailed instructions.

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Unlimited size flowsheets

Only on DESIGN/2000 can you model flowsheets containing essentially unlimited:

unit operations

streams

components

That means also that on most unit operations, you can have unlimited feeds or products. For example, on the distillation unit you can have:

unlimited feeds

unlimited products

unlimited heaters and coolers

unlimited trays

unlimited components

This version has been running for over 1 year, and is available on all our commercial computer systems. You have been using this capability, so there are no coding changes.

For those interested in the computer side of this feature, it is made possible by a dynamic allocation of computer memory. Memory is dynamically released or assigned, as each problem executes on the machine. These operations are controlled with ChemShare's new memory management system. The complexity is even greater on those computers (Univac and CDC) where the program is also heavily overlayed due to non-virtual memories. We have had one customer run an LNG plant with about 150 unit operations, over 250 streams and 10 components. As far as we know, this is the largest commercial simulation ever run.

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AMINE TREATING

As previously announced, only via ChemShare can you look at MEA or DEA treating systems. We are presently running an advertisement in a number of publications, and have reproduced it for your review.

This thermodynamic option has been evaluated by one of the top 5 gas producers in the U.S. and we have been told that the accuracy of our thermodynamic model exceeds what they have used for years, and they plan to use our new technique instead of their own. It is interesting to note, that in ChemShare's 12 years of service, no other thermodynamic and distillation techniques have ever been received with as much initial skepticism. However, after conversations with each user, skepticism has turned into acceptance and understanding.

Remember, questions related to this area should be directed to Dr. John Adams.

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THREE PHASE DISTILLATION

We are presently in the customer testing and evaluation phase of our rigorous three phase distillation column. Test cases are being run at no cost to customers working with us in this phase. We are open for consideration of additional test cases from other customers. Call us if you have specific problems you would like to run.

THREE PHASE FLASH

We are completing the development of a stand alone three phase flash module. We have been testing this module with one of the top 5 engineering and construction companies for the last 3 months, with excellent results. Given VLLE data, the module will compute the three phase region. It is available on version dated 19 JUL 81 and later.

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API SOAVE K-VALUE THERMODYNAMICS

Generally equations such as Soave, Peng-Robinson, and Redlich-Kwong are accurate for mixtures of light hydrocarbons, usually methane through hexane. If H_2S, CO_2, N_2, and/or CO are present, the accuracy is strongly affected unless VLE data are fit to generate binary interaction parameters. The API SOAVE correlation dispenses with this time-consuming extra step since it automatically generates binary interaction parameters based on essentially all of the collected VLE data that is applicable.

The following table lists all of the interactions accounted for by API SOAVE.

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INTERACTION PARAMETERS ACCESSED BY API SOAVE METHOD

Y - yes, parameters stored within API SOAVE correlation

N - no parameters stored

	H_2S	CO_2	N_2	CO
H_2S	-	Y	Y	N
CO_2	Y	-	y	y
N_2	Y	Y	-	Y
CO	N	Y	Y	-
Methane	Y	Y	Y	Y
Ethane	Y	Y	Y	Y
Propane	Y	Y	Y	Y
2-Methylpropane	Y	Y	Y	N
n-Butane	Y	Y	Y	N
2-Methylbutane	N	Y	N	N
n-Pentane	Y	Y	N	N
n-Hexane	N	N	Y	Y
n-Heptane	Y	Y	N	N
n-Octane	N	N	N	Y
n-Nonane	Y	N	N	N
n-Decane	Y	Y	Y	N
Propylene	N	Y	N	N
Cyclohexane	N	Y	N	N
Isopropylcyclohexane	Y	N	N	Y
Benzene	N	Y	Y	N
1,3,5-Trimethylbenzene	Y	N	N	N

API SOAVE also contains correlations to estimate most parameters not shown in the foregoing table.

To specify this thermo option, the commands:

APISOAVEK	for K-Values
APISOAVEH	for Enthalpies
APISOAVED	for Densities

When these commands appear in your GENeral section, DESIGN/2000 immediately scans your components and retrieves the pertinent binary parameters from its internal data base. Parameters not found are estimated in most instances by a correlation. Parameters not so retrieved or estimated are set to zero.

Binary parameters within API SOAVE have been generated from available data over a wide range of conditions. As it enhances accuracy for some sensitive systems to fit data over the specific range of temperatures, pressures, and compositions pertinent to the simulation at hand, ChemShare permits you to enter VLE data for one or more binary pairs. This is easily accomplished via the CHEMTRAN program; such data entry overrides the binary coefficients contained within API SOAVE itself (coefficients for all other binary pairs will be supplied by the API SOAVE correlation).

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CO2 FREEZE PREDICTION IN DESIGN/2000

In recent years lower operating temperatures and high CO2 content found in many gas plants have made the accurate predictions of CO2 solid formation much more important. Most methods which have been in use for a number of years do not take into account the effect of CO2 composition. Since these methods have been quite conservative this has not been a problem. However, with the operating conditions now common in industry many gas plant engineers have recognized the need for a more accurate prediction technique.

In order to meet this need we have implemented in DESIGN/2000 versions 01 JUL 81, and later, the ability to automatically calculate this freeze point on all streams, where it might occur. The run will not be stopped if this condition occurs, but will continue until its normal termination, with a warning message printed for that stream.

To trigger this calculation you need only enter in the GENeral section of DESIGN/2000, the commands:

NATural gas

CO_2 FREeze

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OUR CAPACITY IS TO SERVE YOU.....

.....and we think we will be doing just that by reporting the ratio of heat capacities, C_p/C_v, every time you run an enthalpy option compressor calculation in DESIGN/2000. No additional coding is required to obtain the heat capacity ratio since it will be reported automatically if you use the ENTropy option. The heat capacity ratio for a single stage compressor will appear in the Equipment Summary section (a ratio will be printed for each stage of a multi-stage compressor as the equipment is calculated).

The heat capacity ratio is calculated according to the following relationships:

$$(T_1/T_2) = (P_1/P_2)^{K-1/K}$$

$$K = C_p/C_v$$

where T_2 is calculated from an isentropic compression of the gas from conditions of T_1 and P_1 to pressure P_2. Since the ratio of C_p/C_v is calculated over the pressure range of P_1 to P_2, it is an average.

This feature is available on all program versions with a version date of 01 APR 81 or later (the version date appears in parenthesis at the top of every page of output).

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BRAUN K-10 THERMODYNAMICS IN REFINE

We have installed the K-10 charts for the Braun nomogram equilibrium ratios of hydrocarbons in REFINE. This option is most applicable to crude units, and is similar in application to systems where users presently choose the API (ESSO) option. This option is available on REFINE versions dated 01 Jun 81 or greater.

It is accessed via the input command:

```
DATA K KEY = BRAUN
```


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WHICH METHOD DO YOU PREFER.....

.....to calculate liquid thermal conductivity in REFINE? We ask the questions because you now have three options from which to choose:

1. TEMA NEW
2. TEMA OLD
3. API

TEMA NEW refers to the method described in the TEMA (Tubular Exchangers Manufactureres Association) Handbook, 1972.
TEMA OLD refers to the method described in the TEMA Handbook, 1968.

TEMA NEW treats thermal conductivity as a function of temperature and API gravity, while TEMA OLD and API consider thermal conductivity as a function of temperature only.

The command for selecting your preferred option is:

For TEMA NEW	DAT CON=T
For TEMA OLD	DAT CON=TO
For API	DAT CON=A

The default is TEMA NEW.

These options are available on REFINE versions with a version date of 01 JAN 81 or later (the version date appears in parentheses at the top of each page of output).

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YOU WONT'T NEED ANY MORE GRAPH PAPER.....

.....to plot the results you get from the CHEMTRAN program. When you fit VLE data for non-ideal systems, CHEMTRAN makes the plots for you. Not only that, but you will get new, added results presented in tabular form, too.

Among the advantages you derive from this new output are:

- you can quickly evaluate the accuracy of your data fit.
- you can see the azeotrope points for binary systems and examine the effects of changes in pressure and temperature on the azeotrope.
- you can use the plots to construct McCabe-Thield diagrams.

The easiest way to follow the nature and format of the extra reports is to review an example. The specific example we will examine is a very topical one -- it pertains to fitting VLE data for the azeotrope system of MTBE and methanol. The thermodynamic file created by CHEMTRAN will be subsequently accessed for the DESIGN/2000 simulation of the separation. Of course, MTBE (methyl tetiary-butyl ether) is the gasoline additive projected by many to gain widespread acceptance in the coming year.

Here is the input file for CHEMTRAN, and selected output from the run, to show you some of the plot options.

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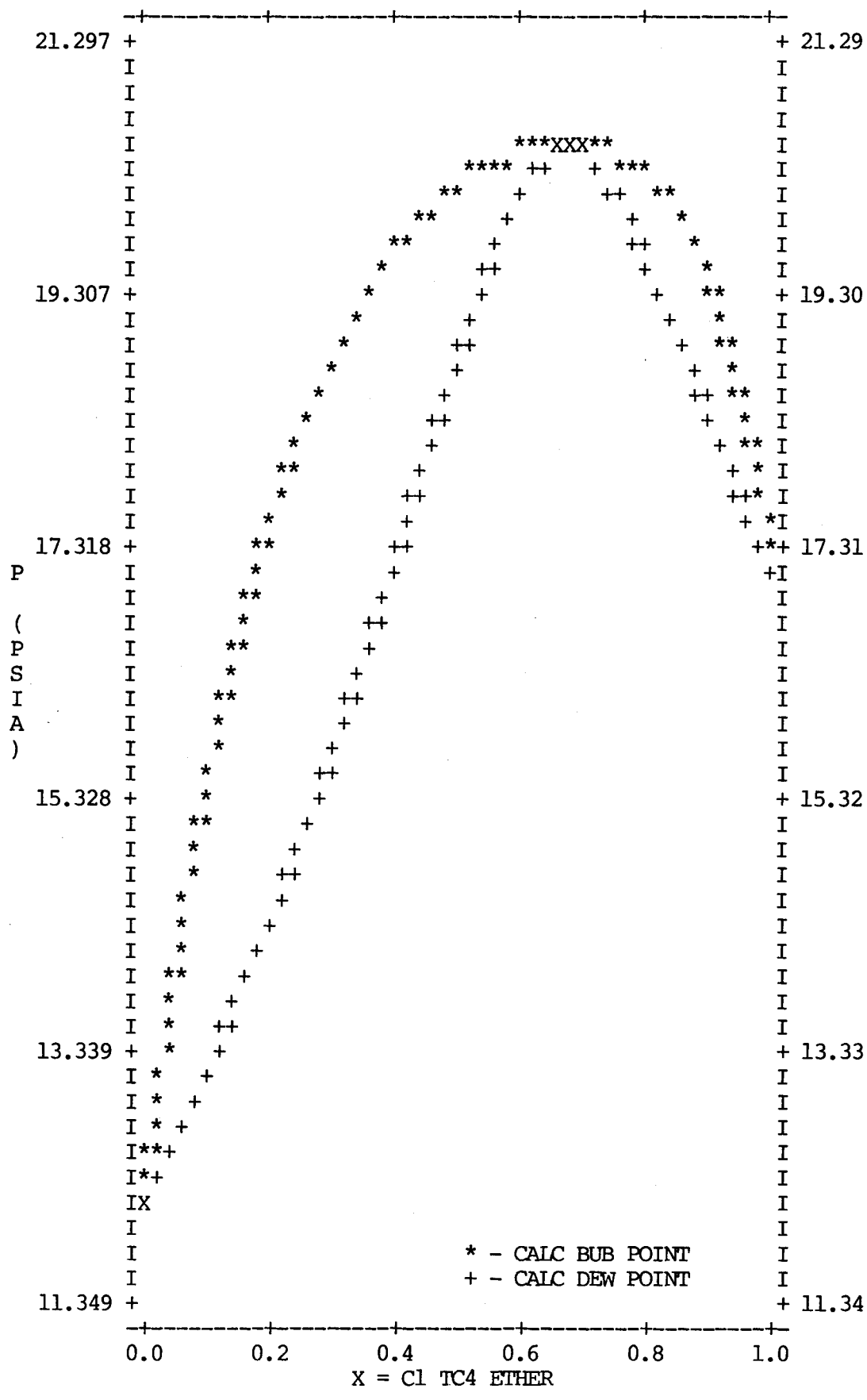
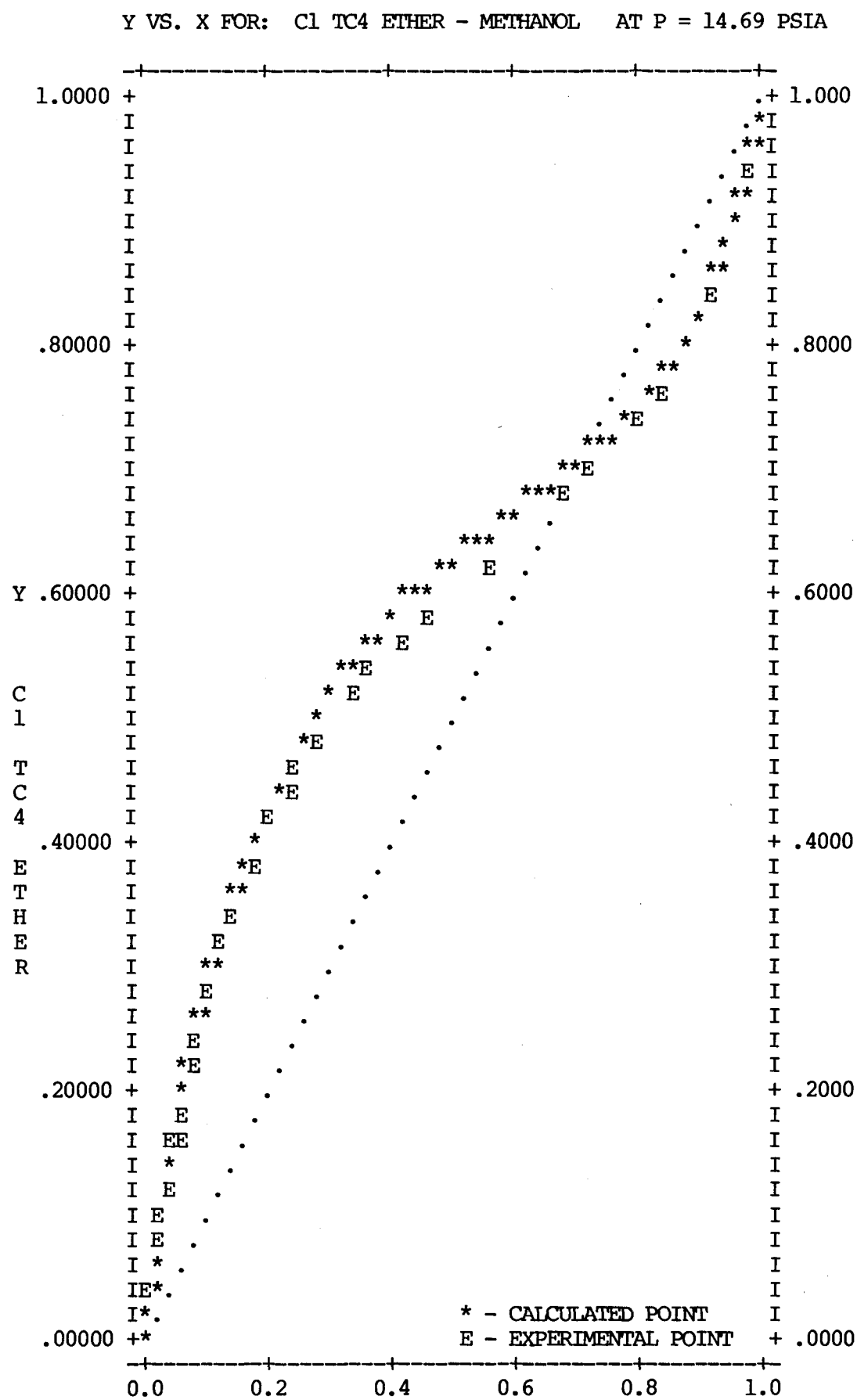
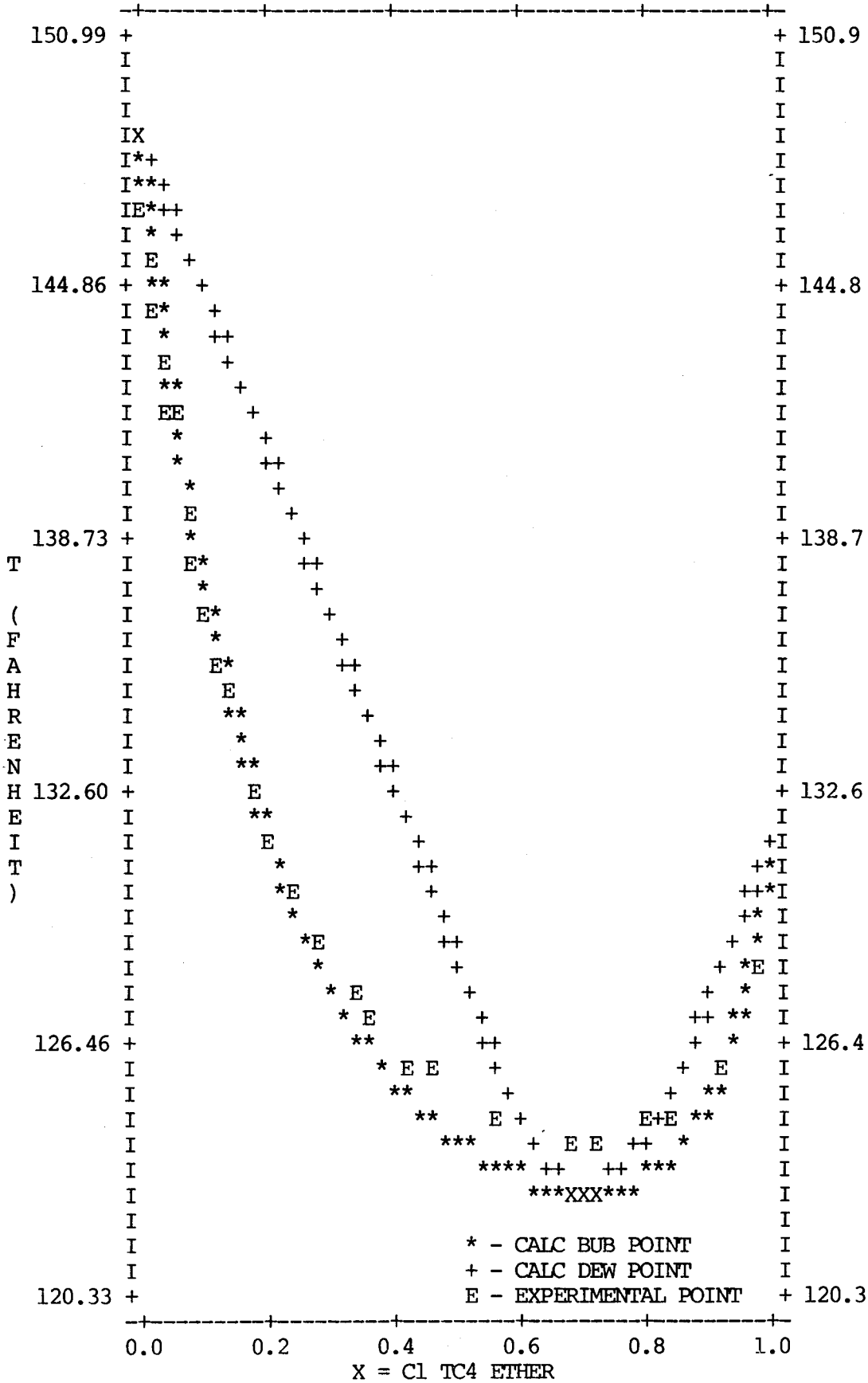
```
* MTBE - METHANOL  (ALM & CIPRIAN, JCEAAX, 25(2) APRIL 1980 PP. 100-103)
COM = 7033,1021
T-Y-X(KPA,C) 7033,1021 = 101.325,
     63.762, .0368, .0095,     62.886, .0776,  .0206,
     62.361, .1023, .0285,     61.845, .1257,  .0360,
     60.964, .1654, .0495,     60.970, .1665,  .0505,
     60.418, .1900, .0595,     59.559, .2283,  .0763,
     59.091, .2488, .0851,     58.406, .2792,  .1016,
     57.596, .3144, .1214,     57.200, .3320,  .1331,
     55.970, .3845, .1743,     55.336, .4133,  .2006,
     54.685, .4408, .2313,     54.369, .4530,  .2470,
     53.703, .4860, .2896,     53.102, .5153,  .3388,
     52.770, .5320, .3678,     52.248, .5620,  .4280,
     51.990, .5790, .4610,     51.460, .6270,  .5651,
     51.232, .6804, .6781,     51.280, .6955,  .7140,
     51.412, .7432, .7970,     51.618, .7650,  .8330,
     52.306, .8485, .9248,     53.517, .9310,  .9790
GRA Y-X(YES,KPA,PRE) 7033,1021 = 50, 75, 101.325, 125, 150, 175, 200
GRA P-X(C) 7033,1021 = 60, 55, 50
GRA T-X(YES,KPA) 7033, 1021 = 50, 75, 101.325,125 ,150, 175, 200
WILSONK
OBJ FUN = 3
END
```

P VS. X FOR: Cl TC4 ETHER - METHANOL AT T = 139.9 DEG F




Y VS. X FOR: Cl TC4 ETHER - METHANOL AT P = 14.69 PSIA
1.0000
.80000
Y .60000
C
l
T
C
4
.40000
E
T
H
E
R
.20000
.00000
1.000
.8000
.6000
.4000
.2000
.0000
* - CALCULATED POINT
E - EXPERIMENTAL POINT
0.0
0.2
0.4
0.6
0.8
1.0
X = Cl TC4 ETHER

T VS. X FOR: Cl TC4 ETHER - METHANOL AT P = 14.69 PSIA



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A WORD ABOUT TESTIMONIALS IN NEWSLETTERS

We believe newsletters are a vehicle to inform you about new program features, technical ideas, and any change to our service.

Unlike other software vendors, we do not believe you want to invest your time in a newsletter that is nothing more than window dressing. Therefore, we do not go after customer testimonials, because testimonials are an advertising gimmick that try to project more than a product has to offer. You will notice that where they were used in the last 2 cases:

1. They had to be retracted, due to inaccuracies and false statements.

2. They contained information from individuals who are clearly misinformed, suggesting that the company, possibly, is also misinformed.

Again, testimonials are an advertising gimmick.

Just to keep our competition in its place, let's review 3 serious and thorough evaluations just recently completed.

1. One of the top 5 refiners: 2 year evaluation using all major vendors. Result: ChemShare leased.

2. One of the top 5 chemical companies: 6 month evaluation to find anyone to solve complex non-ideal extractive distillation. Only solution obtained was via ChemShare.

3. One of the top 5 engineering and construction companies: 4 month evaluation to find software for major petrochemical/ chemical project. Result: ChemShare mounted an in-house to do project.

ChemShare has lots of true success stories, so if you want them, call us.

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HERE A WORKSHOP, THERE A WORKSHOP.....

.....almost everywhere a ChemShare introductory workshop. Why does ChemShare offer so many workshops in all the major process industry centers throughout the U.S. and Canada? Because we want you to get off to the fastest possible start when it comes time for you to use ChemShare programs. And since our workshop frequency has to be high because we regulate the attendance so as to ensure individual attention, we usually have a workshop schedule near you to fit your schedule. Here is a sampling of upcoming workshops. To register, simply complete and return the regisrtation form on your latest workshop notice, or call Karen Ortiz at 713-627-8945.

Los Angeles	June 9
Tulsa	June 10
Houston	June 17
Philadelphia	June 18

By the way, if you have several engineers who would profit by learning about ChemShare programs, it is generally easier and less expensive for you if a ChemShare instructor travels to your place of business. To check into this possiblity, call Karen Ortiz at 713-627-8945 and let her know you are inquiring about an "in-house" workshop.

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