ChemShare

Newsletter No. 201

Month of February, 1982

SELEXOL® Solvent In DESIGN/2000℠

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

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TABLE OF CONTENTS

THE CHEMSHARE CORPORATION 1900 LUMMUS TOWER HOUSTON, TEXAS 77056

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Newsletter No. 201

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Simulation of SELEXOL® Processes Now Possible for Allied Corp's Licensees in DESIGN/2000℠

Allied Corporation's SELEXOL Solvent Gas Purification Department has made their thermodynamic correlations available to their licensees through ChemShare's DESIGN/2000 program. This proprietary solvent is used in many gas processing, refining and chemical applications for selective removal of components, such as CO2 and H2S. ChemShare has many proprietary correlations built into our programs. However these correlations are used primarily for individual companies' own calculations, and occasionally for selected licensees. However, in this case, the arrangement with Allied is unique, in that this is the first time the SELEXOL Solvent technology has been made available in a flowsheet simulation program on an easily accessible commercial basis.

Access to the SELEXOL Solvent correlations is under the direction and control of Allied Corporation. When proper authorization between your company and Allied is established, your company will be given certain passwords in order to access this technology. All passwords are issued by Allied Corp., not ChemShare. In order to request proper authorization, write, do not call, on your company's letterhead to:

Manager Process Development
Allied Corporation
SELEXOL Department
Post Office Box 1021R
Morristown, N. J. 07960

Questions concerning the use of the SELEXOL Solvent thermodynamic correlations in DESIGN/2000 should be addressed to Dr. John Adams at (713) 627-8945. This is available in DESIGN/2000 versions dated (20 Jan. 82) and later.

A reprint of an advertisement that will be appearing in many magazines is given for your reference.

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CO_2 Dehydration

With the permission of the Society of Petroleum Engineers (SPE), and Amoco Production Company we are reprinting for you, in its entirety, a paper by J. W. Best of Amoco Production Company. It was presented at the SPE 56th Annual Technical Conference and Exhibition, held in San Antonio, Texas on October 4 thru 7, 1981.

This article shows how closely you can simulate actual plant conditions when you use experimental data. In this case, Amoco utilized vapor-liquid equilibrium data measured in their laboratories, and then fit it in the CHEMTRAN program. DESIGN/2000 was used for the simulation of the dehydration facility. As can be seen in Table 3, the simulation is extremely close to actual plant performance.

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SPE 10284

SPE
Society of Petroleum Engineers of AIME

Rigorous Computer Simulation of CO_2 Dehydration Facilities

by Jim W. Best, *Amoco Production Company (USA)*

ABSTRACT

The possible development of the Bravo Dome Carbon Dioxide (CO_2) Gas Field located in northeastern New Mexico has led to a detailed study of CO_2 dehydration design using computer simulation. Two commercially available computer programs from the ChemShare® Corporation were used to simulate actual CO_2 dehydration test results. Amoco is currently in the process of using these programs to aid in preliminary design of a full-scale dehydration facility.

INTRODUCTION

In the early 1970's, Amoco Production Company (USA) and others were successful in leasing CO_2 rights underlying more than a million acres of land in northeastern New Mexico in an area called Bravo Dome. The Bravo Dome CO_2 Gas Field is the largest known concentration of CO_2 anywhere in the world and is located approximately 100 miles northwest of Amarillo, Texas. The field encompasses parts of three New Mexico counties: Union, Harding, and Quay.

Carbon dioxide is one of several gases that can be used for enhanced oil recovery of oil bearing formations. The approximately 99 percent pure CO_2 in the Bravo Dome Field has potential application in tertiary recovery of oil in the Permian Basin oil fields of West Texas and eastern New Mexico. Therefore, the possible development of this CO_2 resource has led to the need for designing facilities to process CO_2. The facilities required include CO_2 gas gathering, compression, and dehydration. Dehydration of the CO_2 with triethylene glycol (TEG) is the subject of this paper.

EXPERIMENTAL LABORATORY DATA

The first step in developing an economic process design is to obtain thermodynamic data on the components involved. To that end, experimental CO_2 dehydration data was obtained from a lab analysis conducted at a major southwestern university.

References and illustrations at end of paper

The experimental data collected was vapor-liquid-equilibrium (VLE) data for the CO_2-TEG-H_2O ternary system and the binary CO_2-H_2O system. Some data on the CO_2-TEG system already exists in the literature.

DEHYDRATION FIELD TEST

Although laboratory data is of interest and value, Amoco has always preferred to verify lab data with actual field data, if at all possible. Because of the importance of this facility to our overall CO_2 induced oil recovery process, our management chose to have an actual field test of TEG dehydration of CO_2. The field test conducted at the Bravo Dome CO_2 Field for six months in 1979, was used to obtain operational, corrosion, and production data. The test consisted of producing one well into a 2" and 4" O.D. pipeline, compressing and dehydrating the CO_2 at the test facility approximately 1 1/2 miles away, then injecting the high pressure CO_2 into a well near the test facility. Figure 1 shows schematically the test facility. Figure 2 shows partial data obtained from the dehydration part of the field test.

COMPUTER SIMULATION TECHNIQUE

For verification, the laboratory vapor-liquid-equilibrium (VLE) data for the CO_2-TEG-H_2O ternary system was input into ChemShare® Corporation's CHEMTRAN℠ program. CHEMTRAN℠ is a computer program for prediction and correlation of physical properties for chemicals and chemical mixtures. CHEMTRAN℠ has the capability to regress tabular multicomponent VLE data to unique binary pair interaction parameters for the Peng-Robinson equation of state. The equation of state approach for regressing VLE data relies on the fundamental relationship shown in Table 1. The resultant Peng-Robinson equation of state's enthalpy prediction was also used. The liquid density values were generated by the Yen-Woods correlation, ChemShare's® standard estimation technique for liquid densities. These systems among others are readily available when using ChemShare's® programs.

After the VLE data is entered for different temperatures and pressures, the CHEMTRAN℠ program correlates the mixture data by least square regression analysis. The program evaluates one of several user selected functions, and adjusts the interaction parameters Aij, Aji, Bij, and Bji (binary pair components i and j) until the selected functions shown in Table 2 are best satisfied. The results of the regression analysis can be stored for further use in ChemShare's® DESIGN/2000℠ program.

Generally, only Aij and Aji are adjusted in the data reduction. Parameter Aij is roughly a measure of the strength of the interaction between component i and j. Therefore, the stronger the interaction between component i and j the larger the absolute value of Aij. If the chemical system is close to ideal then the absolute values of Aij will be small. However, for the CO_2-TEG-H_2O ternary system the magnitudes of Aij for each binary pair are large because TEG and H_2O are highly polar and hydrogen bonding molecules.

ChemShare's® DESIGN/2000℠ program rigorously solves heat and material balances for process designs using a user-designated flow scheme and themodynamic option(s). DESIGN/2000℠ in conjunction with the above mentioned CHEMTRAN℠ program yields a unique thermo option to the user.

SIMULATION OF THE GLYCOL CONTACTOR

The interaction parameters discussed above were incorporated into DESIGN/2000℠ through a computer data file. Using DESIGN/2000℠, the TEG dehydration contactor was initially computed using a rigorous column (distillation) module along with the molar flow rate, temperature, and pressure of the lean glycol and CO_2 feed streams as measured during the production field test. The resulting prediction of the distillation module with the complete heat and material balances of the top and bottom product streams was compared to the dehydration field test data. The initial comparison showed the CO_2 concentration in the bottom product (rich glycol) to be approximately 50 percent lower than similar lab data. Also the bottom's temperature was 3°F to 4°F cooler than actual field test data.

The differences between the computer prediction and actual data was assumed to be due to the interaction parameters. Therefore, the CO_2-TEG and the CO_2-H_2O interaction parameters were adjusted to get a better match between the actual CO_2 concentration measured in the bottom product and the computer's prediction.

The problem with the previously determined interaction parameters was believed to be because one or both were temperature or pressure dependent. To confirm whether this variable dependency existed, the CO_2 concentration lab data at different temperatures and pressures, for a 100 weight percent TEG-H_2O solution and a 96.5 weight percent TEG-H_2O solution, was used. The CO_2-TEG interaction parameter was found to vary only slightly with temperature and pressure and, therefore, assumed to be constant for any of Amoco's design conditions. The CO_2-H_2O interaction parameter was found to vary strongly with temperature, but not with pressure. After the temperature dependency of this interaction parameter was accounted for, the CO_2 concentration in the bottom's product and all temperatures and compositions simulated by the program came into close agreement with the test and lab data. Table 3 shows the comparison of computer results and the actual data.

CONCLUSIONS

The detailed study of CO_2 dehydration using the computer has shown that ChemShare® Corporation's CHEMTRAN℠ and DESIGN/2000℠ computer programs are capable of simulating a CO_2 dehydration facility. The CHEMTRAN℠ program is a valuable tool for design because of its capability to allow experimental lab data to be integrated into physical properties, as calculated by the Peng-Robinson equation of state; for further use in the DESIGN/2000℠ program.

NOMENCLATURE

CO_2	Carbon Dioxide
VLE	Vapor-Liquid-Equilibrium Data
K-Value	Vapor-Liquid Equilibrium Constant
Aij	Interaction Parameter
T	Temperature
P	Pressure
Y	Vapor Fraction of a Component
X	Liquid Fraction of a Component
O.D.	Outside Diameter
Lb.	Pound Mass
MMSCF	Million Standard Cubic Feet

REFERENCES

1. Engineering Services©, ChemShare 1978, Guide to Solving Process Engineering Problems by Simulation; The ChemShare Corporation® 1900, Lummus Tower; Houston, Texas.

TABLE 1

EQUATIONS OF STATE

$$Y_i \phi_i^{vap} (T, P, Y_i; A, B) = X_i \phi_i^{liq} (T, P, X_i; A, B)$$

WHERE:

ϕ_i^{vap} = FUGACITY OF COMPONENT I IN THE VAPOR CALCULATED FROM EQUATION OF THE STATE

Y_i = MOLE FRACTION OF COMPONENT I IN VAPOR

ϕ_i^{liq} = FUGACITY OF COMPONENT I IN THE LIQUID CALCULATED FROM EQUATION OF STATE

X_i = MOLE FRACTION OF COMPONENT I IN THE LIQUID

PARAMETERS A AND B ARE USED TO ADJUST THE FUGACITY EQUALITY TO FIT EXPERIMENTAL DATA. THE PARAMETER B IS USED TO ACCOUNT FOR TEMPERATURE DEPENDANCE.

K-VALUE

$$K = \frac{Y_i}{X_i} \text{ (IDEAL GAS)}$$

ADJUSTED BY A AND B: $K = \frac{Y_i \phi_i^{vap}}{X_i \phi_i^{liq}}$ (NON-IDEAL GAS AND SOLUTIONS)

TABLE 2

OBJECTIVE FUNCTION

K-VALUES $\quad I = 1 \left[1 - \frac{(K_i)\,calc}{(K_i)\,exp}\right]^2 = 0$

K-VALUES WEIGHTED BY Y_i $\quad I = 1 \left[1 - \frac{(K_i)\,calc}{(K_i)\,exp}\right]^2 Y_i = 0$

TABLE 3

COMPARISON OF SIMULATED VS. ACTUAL DATA

TOP PRODUCT STREAM (DRY CO_2)	COMPUTER SIMULATED	ACTUAL
TEMPERATURE, °F	101	102
WATER CONTENT, LB. H_2O/MMSCF	10.4	11
CO_2 FLOWRATE, LB. MOL/HR.	107.0	107.1
H_2O FLOWRATE, LB. MOL/HR.	.0236	.0249
BOTTOM PRODUCT STREAM (RICH GLYCOL)		
TEMPERATURE, °F	99.37	98
CO_2 FLOWRATE, LB. MOL/HR.	.393	.345
H_2O FLOWRATE, LB. MOL/HR.	.305	.304
CO_2 CONCENTRATION, LB. MOL CO_2/LB. MOL SOL	.213	.188

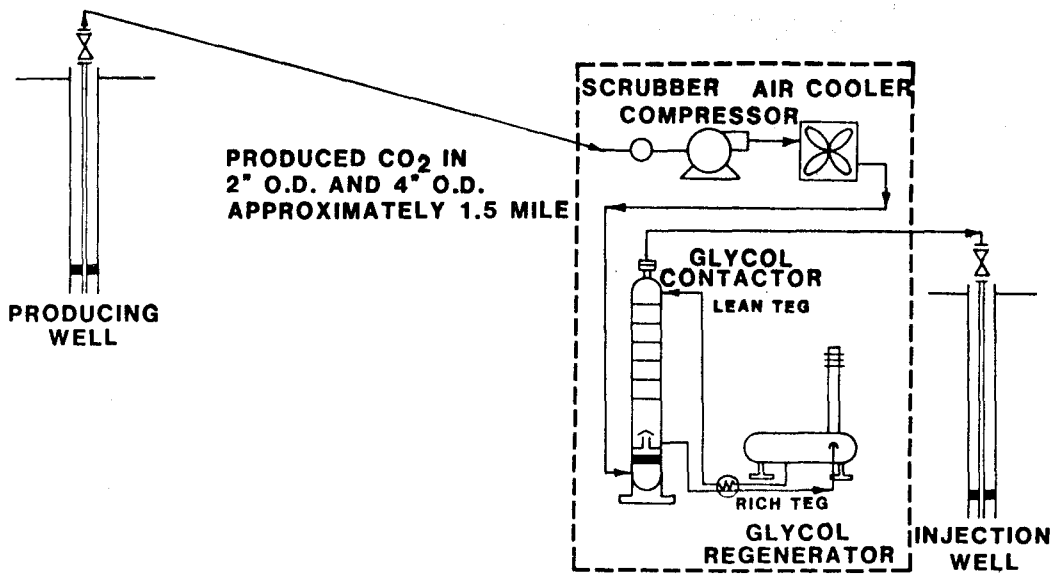

FIGURE 1 **DEHYDRATION FIELD TEST DIAGRAM**

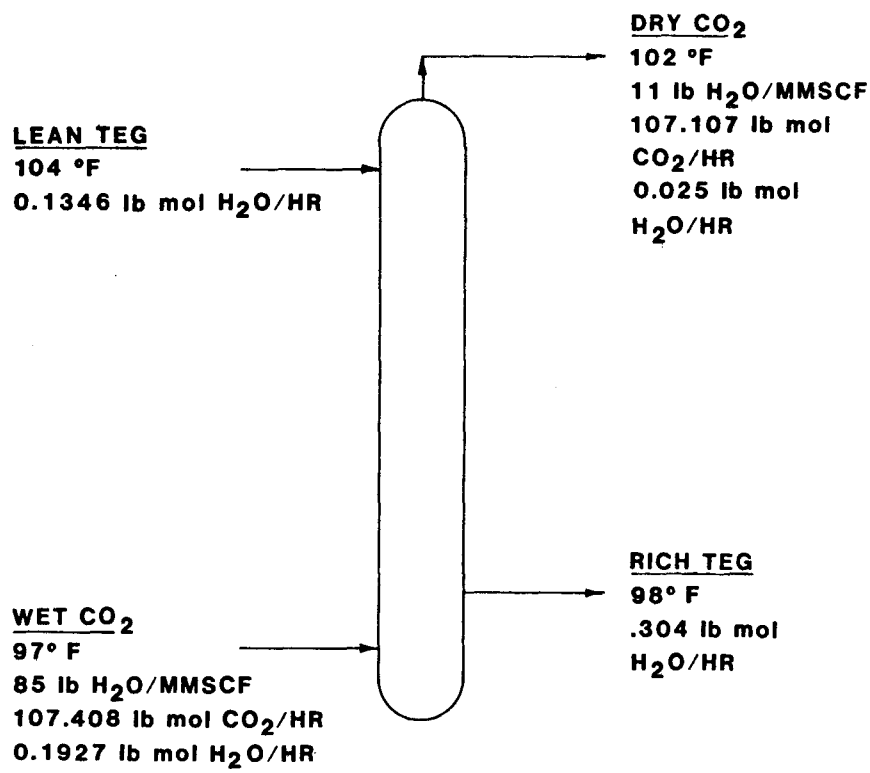

FIGURE 2 **CO_2-TEG CONTACTOR**

FORTRAN In DESIGN/2000

ChemShare is pleased to announce that it now has the ability to allow users to enter FORTRAN commands directly as part of the input for DESIGN/2000. This capability results from the development by ChemShare of a FORTRAN processor linked directly with DESIGN/2000. This new system will eliminate the several steps associated with writing separate FORTRAN subroutines to create ADD modules and linking them into DESIGN/2000. Because of this feature, you will be able to model almost anything you many want including reactors, pressure drop/line sizing calculation, economics or more complex control loops.

The level of FORTRAN is such as to allow the user the ability to use subroutinges, function subroutines, FORTRAN mathematical libraries, and subroutines available in DESIGN/2000. This feature is unique, since the FORTRAN processor is an integral part of DESIGN/2000, not external to DESIGN/2000. Since the processor is a part of DESIGN/2000, the machine language code that actually does the process calculations for you is created quickly and efficiently.

This feature is only available on our PRIME computer systems at this time. We will be moving this capability over to other computer systems over the next year. A sample problem illustrating the use of this capability is shown below.

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```
*INPUT EXAMPLE FOR INLINE FORTRAN
ADD8=SEP,1,-2,-3,USE BLOCK3,NEQP=1
EQP=.5
GEN,COM=3,4,5
FLO1=5,90,5
TP1=98,190
FORTRAN
BLOCK3=1,MAIN,CHACMP
START LIBRARY
      SUBROUTINE MAIN ( NIN,    NOUT,   NOCOMP, NEQP,   NDSP,
     &          SIVPFR, SITEMP, SIPRES, SIENTH, SIMOLE, SICOMP, SIKV,
     &          SOVPFR, SOTEMP, SOPRES, SOENTH, SOMOLE, SOCOMP,
     &          SOKV,   EQPAR,  DESPAR, AMW,    ATB,    IDCOMP  ,
     *          ISTOP,  KTRACE, NCP)
C--
      DIMENSION SIVPFR(NIN), SITEMP(NIN), SIPRES(NIN), SIENTH(NIN),
     &          SIMOLE(NIN), SICOMP(NOCOMP,NIN), SIKV(NOCOMP,NIN)
      DIMENSION SOVPFR(NOUT), SOTEMP(NOUT), SOPRES(NOUT), SOENTH(NOUT),
     &          SOMOLE(NOUT), SOCOMP(NOCOMP,NOUT), SOKV(NOCOMP,NOUT)
      DIMENSION EQPAR(NEQP), DESPAR(NDSP), AMW(NOCOMP), ATB(NOCOMP),
     &          IDCOMP(NOCOMP)
C--
C--
C-----------------------------------------------------------------------
C--    SET FLOW COMPONENT 3 TO A FRACTION OF COMPONENT 4.  FRACTION
C--    IS FIRST PARAMETER IN EQPAR VECTOR
C--
      CALL CHACMP (NOCOMP,NIN,SICOMP,EQPAR(1))
      CALL  DB  ( NINX, NOUTX, NOCOMP, NEQP, NDSP, SIVPFR, SITEMP,
     &                 SIPRES, SIENTH, FLOW(I), X(1,I), SIKV, SOVPFR(I),
     &                 SOTEMP(I), SOPRES(I), SOENTH(I), SOMOLE(I),
     &                 SOCOMP(1,I), SOKV(1,I), EQPAR, DESPAR )
      RETURN
C--
      RETURN
      END
      SUBROUTINE CHACMP (NC,NI,C,FRACT)
      DIMENSION C(NC,NI)
      C(1,1)=FRACT*C(2,1)
      RETURN
      END
STOP LIBRARY
END
```


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Newsletter No. 201

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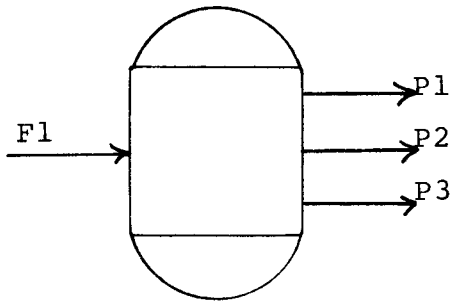
Reverse Material Balance



Suppose you are an operating company making products P1, P2, P3 from F1. The compositions of all products and feeds are known and are accurately monitored. However, due to inaccuracies of typical flowmeters, the measured flowrates of the products may be off as much as 5 to 10%. It would be nice to be able to check the flowmeters based on product compositions and feed flowrates, so as to calibrate these meters.

ChemShare has created a unit operation which will back-calculate the product flowrates from the compositions of the products and the feed, plus the feed flowrate. With these flowrates, the accuracy of the flowmeters can be determined. If your flowsheet involves several stages of separation, you can do a better job of optimizing when you are working with more accurate product flowrates.

In the following example a partially condensed organic stream is separated into its three constituent phases. An accurate composition analysis is available on all streams, but the only known flowrate is the feed stream. This information is summarized below.

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STREAM NUMBER	1	2	3	4
MOLE FRACTIONS:				
HYDROGEN	0.5000	0.9315	0.0031	0.0025
METHANOL	0.0500	0.0076	0.0425	0.1604
WATER	0.2000	0.0237	0.0323	0.8093
TOLUENE	0.2500	0.0372	0.9221	0.0278
TOTAL	1.0000	1.0000	1.0000	1.0000
TOTAL FLOW, LBMOL/HR	100.0	??????	??????	??????

ECHO PRINT OF INPUT DATA

```
*MASS BALANCE ADD MODULE WITH 4 COMPONENTS AND 3 PRODUCTS
ADD1=SEP,1,-2,-3,-4,USE ADD3,NEQP=13
EQP=1,
.9315, .0076, .0237, .0372,
.0031, .0425, .0323, .9221,
.0025, .1604, .8093, .0278,
GEN,COM=1,1021,62,41
FLO(FRA)1=.50,.05,.20,.25
TOT FLO 1=100
TP(C)1=25,14.7
END
```

This unit operation is currently available as an ADD module, but could become a permanent equipment module if there is sufficient interest. So call Bill Hensley at (713) 627-8945 if you have any questions.

A background note on this module: The operating company who asked us to review this problem said they had talked to a competitor of ours, who claims to have the best darn, gee whiz, simulation program. But due to a lack of technical skills, interest, or capabilities, they apparently could not solve this problem. Sometimes, being second at the starting gate doesn't mean you'll finish in second place.

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Newsletter No. 201

Month of February, 1982

Output Units in CHEMTRAN

The capability of specifying output units (metric, SI, etc.) has now been added to CHEMTRAN. The commands are the same as in DESIGN/2000 and can be placed anywhere in the input. They are:

```
SI UNITS OUT
METRIC UNITS OUT
PREssure UNITS OUT =
TEMperature UNITS OUT =
ENThalpy UNITS OUT =
```

This is available in CHEMTRAN versions dated (01 Mar 82) and later.

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ChemShare Goes Back To School

Over the past 3 years, ChemShare has made its software available free of charge to a number of universities. The programs have been used for educational purposes in graduate and undergraduate courses, with essentially no technical assistance from us. We will continue to add universities each year. We thought that if any of our readers are alumni of these institutions they might be interested to know that our programs are installed at their university.

Louisiana State University
Texas A & M University
Rice University
University of Alabama
University of Newcastle
University of Oklahoma
University of Pennsylvania
University of South Carolina
University of South Florida
University of Singapore
University of Utah
Virginia Polytechnic Institute

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Newsletter No. 201

Month of February, 1982

Request for Information

Newsletters

_____ April '81
_____ May '81
_____ August '81
_____ October '81
_____ December '81
_____ February '82

Advertisement Reprints

_____ MEA/DEA
_____ MTBE - Methanol
_____ REFINE End Points
_____ Gasohol
_____ SELEXOL Solvent

Sample Problems

_____ Gas Processing
_____ Refining
_____ Chemical

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(DESIGN/2000 and CHEMTRAN)
_____ Updates (Rev. Mar '81)

Change of Address

_____ Add _____ Delete _____ Change: Name _____

Company: _____

Address: _____

City: _____ State _____ Zip _____

Telephone: _____

Mail to: Sales Secretary
ChemShare
Post Office Box 1885
Houston, Texas 77001

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