CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 27

Fall 1988

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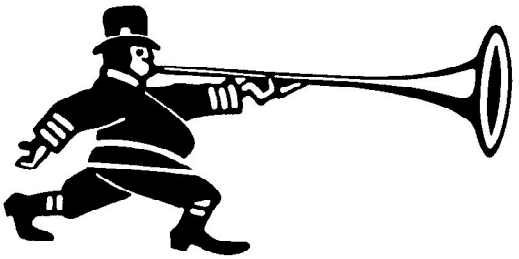


ANNOUNCEMENTS

Foundations of Computer-Aided Process Design (FOCAPD '89), July 9-14, 1989

The third FOCAP-D Conference will take place in the summer of 1989 in Snowmass, Colorado.

Nine sessions are planned. Conference themes include: Design Theory and Methodology, Artificial Intelligence, New Design Environments, Process Synthesis, Mathematical Techniques, Process Simulation and Analysis, Applications of Supercomputers, Chemical Product Design, and Future Outlook.

For further information contact the Conference Chairman:

Jeffrey Siirola
Eastman Kodak Company
P.O. Box 1972
Kingsport, TN 37662
(615) 229-3069

or Conference Vice Chairman:

Ignacio E. Grossman
Dept. of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
(412) 268-2228

CACHE Anthology of On-Line Computer Applications

The CACHE Anthology of On-Line Computer Applications in the Undergraduate Chemical Engineering Laboratory is now available. Chemical engineering department chairs received their copies in September.

Approximatcly 20 write-ups covering the major areas of the traditional chemical engineering laboratory, i.e., thermodynamics, transport, chemical reactors, and process control will be included in this single volume. The table on the next page lists the contributors, their schools and the titles of the descriptions.

More than half of the write-ups focus on the fundamental chemical engineering phenomena that are involved. In each case the authors show how an on-line computer, usually an inexpensive microcomputer with off-the-shelf input/output cards, can be used effectively to take data from a process or operating unit, analyze these raw results using theory at the level of a typical undergraduate lecture course, and display the final results. Particular details concerning construction of the experimental unit and instrumentation are included to help someone duplicate the experiment at another school. In most cases, the type of computer used is relatively unimportant and the software is either easy to develop, can be obtained from the authors, or is available as a commercial package. These features make program development quite simple.

Ordering information is available from the CACHE main office. Other information may be obtained from either of the volume editors:

Prof. Duncan Mellichamp
Dept. of Chemical Engineering
Massachusetts Institute of Technology
66-562
Cambridge, Massachusetts 02139

Prof. Ali Cinar
Illinois Institute of Technology
Chemical Engineering Dept.
IIT Center
Chicago, Illinois 60616

CACHE Anthology of On-Line Computer Applications in the Undergraduate Chemical Engineering Laboratory

Author/School	Title of Experiment
L. W. Bezanson Arizona State Univ.	a) Compression & Expansion Characteristics of Air b) Vapor Pressure Determination of Water
R. A. Buonopane Northeastern Univ.	a) Humidification in a Packed Column b) Concentric Tube Heat Exchanger c) Aeration of Water Using a Kenics Static Mixer
Ali Cinar ITT, Chicago	a) Alarm System b) Control of Two Heat Exchangers in Series
M. J. Cooney & K. A. McDonald	a) Steady-State & Transient Analysis in Fermentation
D. A. Crowl Wayne State Univ.	a) Valve Dynamics
K. A. Debelak et al. Vanderbilt Univ.	a) On-Line Data Acquisition for an Isothermal Batch Reactor b) Residence Time Studies in a CSTR
M. Ellis & K. Jensen Univ. of Minnesota	System Dynamics Identification
J. C. Hassler Univ. of Maine	Continuous Stirred Tank Systems: Multiple Configuration with Level or Level/Temperature Control
R. H. Heist & T. Olsen Univ. of Rochester	a) Unsteady-State Heat Transfer in a Sphere b) Ion Exchange
D. Karman Univ. of New Brunswick	Unsteady-State Heat Transfer in a Cylinder
J. Keller & H.-J. Reinhart ETH-Zurich	Control of a Discontinuous Process
S. Rohani Univ. of Saskatchewan	Surge Tank Control
D. Smith Brigham Young Univ.	Pressure Loss in Pipes and Fittings
M. Stadtherr & R. Masel Univ. of Illinois	Air Flow Temperature Control
D. C. Williams Auburn Univ.	Experiments with Two Gas Storage Tanks in Series

THE CASE FOR MACROS

Lotus 1-2-3 Subroutines

by Edward M. Rosen
Monsanto Co., St. Louis, Missouri

The usefulness of spreadsheet programs in chemical engineering education is well recognized by the CACHE Corporation and the Education and Accreditation Committee of AIChE.[1] It is therefore of interest to fully explore the capabilities of a widely-used spreadsheet program such as Lotus 1-2-3.

Although \ X macro commands of Lotus 1-2-3 were available in previous releases, Advanced Macro Commands[2] have only become available since Release 2. These macro commands are more clearly named than the old \ X macro commands which makes it easier to follow a listing of them.

Since learning a new capability takes time and effort it is fair to ask whether it is worthwhile, especially if a calculation can be carried out in another way, say, using FORTRAN or BASIC. Though the answer depends on the job, system availability and a host of other factors, the advanced macro capability of Lotus 1-2-3 only takes a day or so to learn.

One of the limitations of the standard worksheet is that it does not allow the "loop within loop" calculation which arises so often in chemical engineering. However with macros this limitation is removed and the capability to use subroutines in some of the same ways as in FORTRAN is possible.

There are some differences, however, in using subroutines in Lotus 1-2-3 as compared to FORTRAN. Whether arguments are passed or not, the subroutine can directly address any of the cells in the spreadsheet. Although arguments can be passed to the subroutine, the results from the subroutine cannot be passed to a relative location in the spreadsheet. Instead the results must be picked up from cells designated by the subroutine.

These ideas are illustrated in Fig. 1 which shows the coding for a general purpose subroutine ROOTX based on Wegstein's method[3] for solving a one-dimensional equation of the type

$$x=f(x)$$

The subroutine operates in two modes. If the code (cell X6) is set to 0, then the working cells (X7 to X16) are cleared and control is returned to the calling routine. If the code (cell X6) is set to 1, then the routine will return a new x for each pair of values xn and f(xn) supplied as arguments which are passed to cells X4 and X5 using the DEFINE command keyword. Note that the upper and lower bounds on the slope are set in cells X1 and X2.

The calling program is given by the \ q macro. It is set up to solve either of two problems determined by location S6 (PROB). The arguments passed to the subroutine, S9, xn and S10, f(xn), are specified in the call to the subroutine, i.e., {ROOTX S9,S10}. The new value of x is picked up from location X4 of the subroutine and passed to location S9 with the {LET S9,X4} command. The convergence criterion is given in the calling program and can be problem dependent.

The cells above the \ q macro are data and scratch calculations for the two problems solved. The first problem (PROB 0) is given by Myers and Seider,[4] p. 454, and was solved in a standard spreadsheet manner in Rosen.[5] The problem is to find the volume in an equation of state:

$$v = -P*v** 3/a+R*T*v** 2/a+b*Pv** 2/a+b$$

Starting with v=10, the answer is v=224.4454 after 14 iterations. Calculations from this problem is shown in Term1..Term3 above EVAL.

The results of the second problem, shown above ROOTX and EVAL1 (Term1..Term5), is given by Reklaitis (p. 569). The problem is to find T (deg K) that satisfies an equation of the form

$$T=F(T)$$

The data to evaluate F(T) are given in the reference or can be obtained from the figure. The answer after 4 iterations starting with T=600 K is 742.80 K. Reklaitis gives 738.88 K.

Alhough macros were originally designed to simply allow the storage of keystrokes so they would not have to be repeated in routine applications, they allow a great deal of freedom in performing chemical engineering calculations. Consider using them in your own calculations.

References

1 AIChE, Education and Accreditation Committee, *Evaluating Programs in Chemical Engineering*, August 1, 1988.

2 Lotus, *1-2-3 Reference Manual, Release 2.*

3 Lotus, Henley, E. J. and E. M. Rosen, *Material and Energy Balance Computations*, John Wiley, New York (1976).

4 Myers, A. L. and W. D. Seider, *Introduction to Chemical Engineering and Computer Calculations*, Prentice Hall, Englewood Cliffs (1976).

5 Lotus, Rosen, E. M. and R. N. Adams, "A Review of Spreadsheet Usage in Chemical Engineering Calculations," *Computers and Chemical Engineering*, Vol. 11, No. 6, pp. 723-736 (1987).

6 Lotus, Reklaitis, G. V., *Introduction to Material and Energy Balances*, John Wiley, New York (1983).


```
        a          1351000
        b            38.64
        P atm           50
        R             82.06
        T K          173.15


S9:     xn         742.7960
S10:    f(xn)      742.7960

        Term1      -368.726
        Term2      520.4101
        Term3      70.76179

        PROB              1


EVAL    {LET S12,S2-S3*S9*S9*S9/S1}
        {LET S13,S4*S5*S9*S9/S1}
        {LET S14,S2*S3*S9*S9/S1}
        {LET S10,S12+S13+S14}


        Term1      763.9411
        Term2      35968.30
        Term3      48790.69
        Term4      29226.23
        Term5      6026.382


EVAL1   {LET S25,698.15+26907.1*1.2/490.773}
        {LET S26,0.5591*(S9^2-698.15^2)}
        {LET S27,7.0155E-4*(S9^3-698.15^3)}
        {LET S28,4.3718E-7*(S9^4-698.15^4)}
        {LET S29,1.E-10*(S9^5-698.15^5)}
        {LET S10,S25-(S26-S27+S28-S29)/490.773}
```

```
upper     X1: 0.8
lower     X2: -9

xn        X4: 742.7960177
fn        X5: 742.79667168
code      X6: 1
counter   X7: 4
x1        X8: 742.38719496
f1        X9: 742.99079659
x2        X10: 742.79464505
f2        X11: 742.79667168
slope     X12: -0.4764384809
t         X13: 0.6773055653
t*delta   X14: 0.0013726472
term1     X15: 0.4074500977
denom     X16: 0.4074500977


ROOTX     X21: '{DEFINE X4:VALUE,X5:VALUE}
          X22: '{CALC}
          X23: '{IF X6=0}{BRANCH X25}
          X24: '{BRANCH X27}
          X25: '/CX6~X7..X16~
          X26: '{RETURN}
          X27: '{LET X7,X7+1}
          X28: '{LET X8,X10}
          X29: '{LET X9,X11}
          X30: '{LET X10,X4}
          X31: '{LET X11,X5}
          X32: '{LET X15,@ABS(X10-X8)}
          X33: '{IF X15>0}{BRANCH X36}
          X34: '{LET X16,1}
          X35: '{BRANCH X37}
          X36: '{LET X16,X10-X8}
          X37: '{LET X12,@MIN(X1,@MAX(X2,(X11-X9)/X16))}
          X38: '{LET X13,1/(1-X12)}
          X39: '{LET X14,X13*(X11-X10)}
          X40: '{LET X4,X4+X14}
          X41: '{IF X7=1}{LET X4,X5}
          X42: '{RETURN}
```

```
\q      {LET X6,0}                          Clear
        {ROOTX S9,S10}
        {LET X6,1}                          Set ROOTX
R47:    {IF S16=0}{BRANCH R50}              Select Prob 1 or 2
        {EVAL1}
        {BRANCH R51}
R50:    {EVAL}
R51:    {IF @ABS(S9-S10)<1.E-6}{BRANCH R55} Test
        {ROOTX S9,S10}                      Get new x
        {LET S9,X4}                         Set S9
        {BRANCH R47}                        Evalute function
R55:    {CALC}                              Complete
```

Fig 1.

General Purpose MACRO Subroutine ROOTX

PERSONAL COMPUTER SOFTWARE: EDUCATIONAL DEALS WITH SPECIAL PRICING

by Michael B. Cutlip

It is always difficult to keep abreast of new developments in personal computer software. I have listed several of the major software suppliers who have special educational programs with significant discounts for faculty and students. This may be of some interest to those who wish to purchase personal copies or obtain copies for evaluation. This material is provided as information only and does not indicate CACHE approval of any of the products. Information was in effect as of October 1988.

Ashton-Tate
Educational Marketing Dept.
20101 Hamilton Avenue
Torrance, California 90502-1319
(213) 538-7725 or 7726

Educational Support Program. Faculty are requested to call (800) 437-4329 ext. 3407 to find out if the campus bookstore or computer center carries Ashton-Tate products with educational prices. If products are not available locally, then institutional orders will be accepted at the above address. Products include: dBase III+ 1.1 ($195), Framework III ($99), MultiMate 3.3 ($85), Multimate Advantage II 1.0 ($125), Master Graphics ($200), dBase Mac 1.01 ($99), FullWrite Professional (Mac) ($99).

Borland International
Educational Sales Dept.
P. O. Box 660001
Scotts Valley, California 95066-0001
(408) 438-8400 (educational sales)

Scholar Program. This program provides for direct sales of Borland products to departments, faculty of students of accredited institutions in the U.S. or Canada, when the product will be used in conjunction with a class. Contact Borland for details. Programs include: Turbo Pascal 4.0 ($39.95), Pascal Tutor 4.0 ($29.95), Turbo Prolog 2.0 ($44.95), Turbo Basic ($33.95), Turbo C ($44.95), Reflex ($49.95), Quattro ($44.95), SideKickPlus ($49.95), SuperKey ($39.95), Eureka ($39.95), and many others including some for the Mac.

Microsoft Corp.
Box 97017
Redmond, Washington 98073-9717
(800) 227-4679

Their Academic Excellence Program which used to provide faculty the opportunity of evaluating Microsoft products at a fraction of their normal price *has been discontinued.* A new program is being developed but details are not yet available. Sales of languages direct to universities carry an approximate 45% discount.

Chambers International Corp.
5499 N. Federal Highway
Suite A
Boca Raton, Florida 33487
(407) 997-9444

Sales Program. This company limits its marketing to academics and one can easily obtain detailed information on their software. A variety of companies use Chambers for educational offers. Typical software includes: DataPerfect ($125), Drafix 1 Plus ($160), Enable 2.0 ($175), Norton Utilities 4.0 ($75), SuperCalc$ Rel. 1.1 ($135), WordPerfect 5.0 ($135), TK! Solver Plus ($150), Volkswriter Scientific ($75), many others for IBM, Mac and Apple.

WordPerfect Corp.
1555 N. Technology Way
Orem, Utah 84057
(801) 255-5000 (educational sales)

WordPerfect has a Student Software Program where both faculty and students can purchase directly from the company. Attractive multiple user costs and network support are available. Software includes: WordPerfect 5.0 ($135), DataPerfect ($125), PlanPerfect ($99), WordPerfect Executive ($79), WordPerfect 1.0 for Mac ($99).

CAI IN ADVANCED PROCESS CONTROL

by Gomatam R. Arulalan, Sanjay Kumar, Pradeep B. Deshpande
University of Louisville

The following is an excerpt of an article written by Drs. Arulalan, Kumar and Deshpande. It describes a set of computer programs for instruction in advanced process control that complement the design concepts covered in *Computer Process Control with Advanced Control Applications* by Deshpande and Ash, *Multivariable Control Methods,* and *Distillation Dynamics and Control,* both by Deshpande. The topics include open loop and closed-loop response evaluations, process identification, optimal tuning of PID-type controllers, digital controller design procedures for deadbeat control, internal model control (factorization method) Dahlin algorithm, Smith Predictor, feedforward control, simplified model predictive control, internal model control (predictive control formulation), and dynamic matrix control. The programs will be useful not only to educators, but also to control engineers in industry.

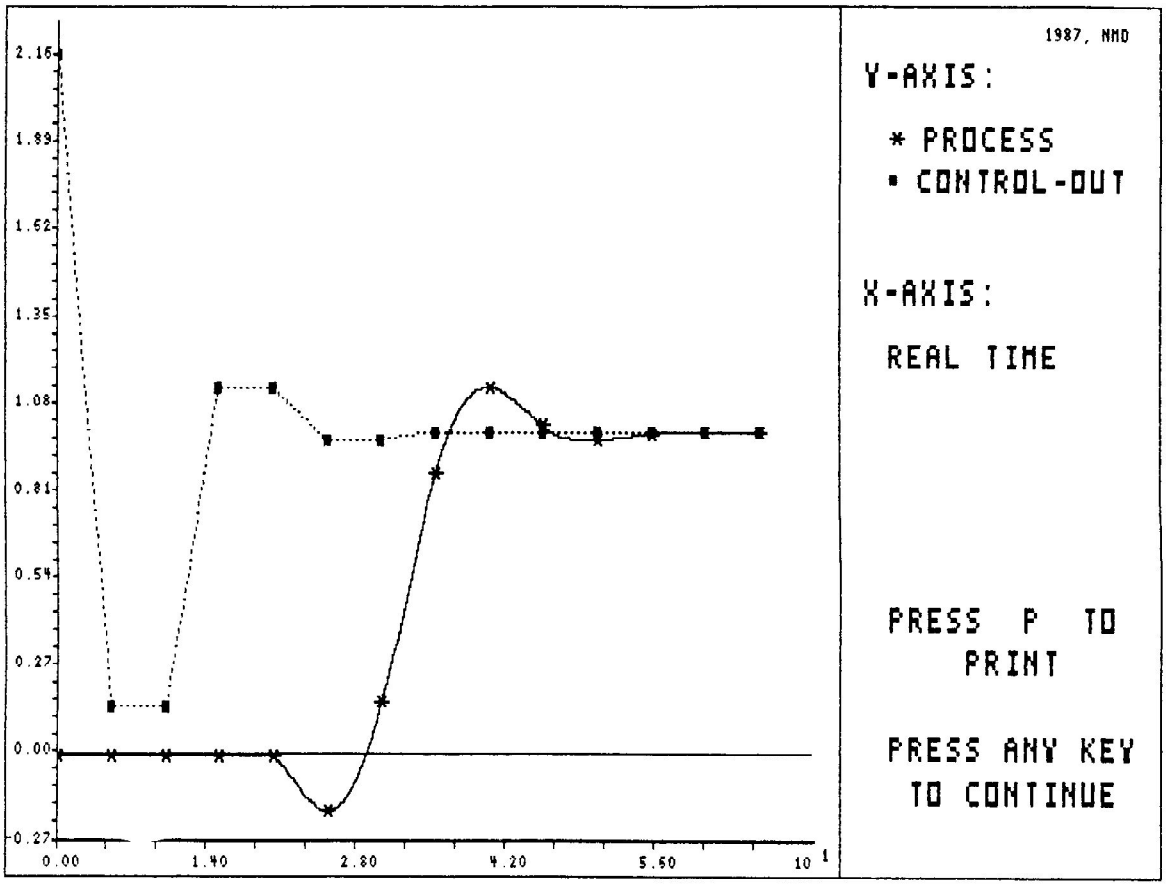
Dr. Arulalan is currently with Fluor-Daniel Company in Greenville, South Carolina and Dr. Kumar is with Exxon Chemical Company in Baytown, Texas.

The CAI software consists of fifteen programs, twelve of which are for single- input single-output (SISO) systems and three of which are for multivariable systems. The hardware requirements are an IBM PC/AT with 640K memory and hard disk, monochrome display and Hercules Graphics card (or IBM color display and IBM color graphics card), math coprocessor and IBM Quietwriter printer. Compatible systems will also run the software. The operating system is MS DOS 3.1.

Figure 1 is an example of graphics output from the program.

The set of programs include:

OPEN	Open-loop response.
PROCESID	Process identification by random search method.
CLOSE	Closed-loop response with PID controller.
RANOPT	Optimized tuning of PID controller by random search procedure.
LEASTOPT	Optimized tuning of PID controller by lease squares optimization.
FEEDFOR	Combined feedback/feedforward control.
SMITH	Smith predictor.
SVIMCFAC	Single variable internal model control (factorization method).
SVSMPC	Single variable simplificd model predictive control.
SVFMC	Single variable forward modeling control.
SVIMCPRE	Single variable internal model control by predictive control formulation.
SVDMC	Single variable dynamic matrix control.
MVIMCPRE	Multivariable internal model control by predictive control formulation.
MVDMC	Multivariable dynamic matrix control.
MVSMPC	Multivariable simplified model predictive control.




```
SUM OF ERROR SQUARED =          27.1550900
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1 - NEW SETPOINT/DISTURBANCE
2 - NEW TUNING PARAMETER
3 - NEW MODELING ERRORS
4 - NEW PROCESS
5 - EXIT
4
```
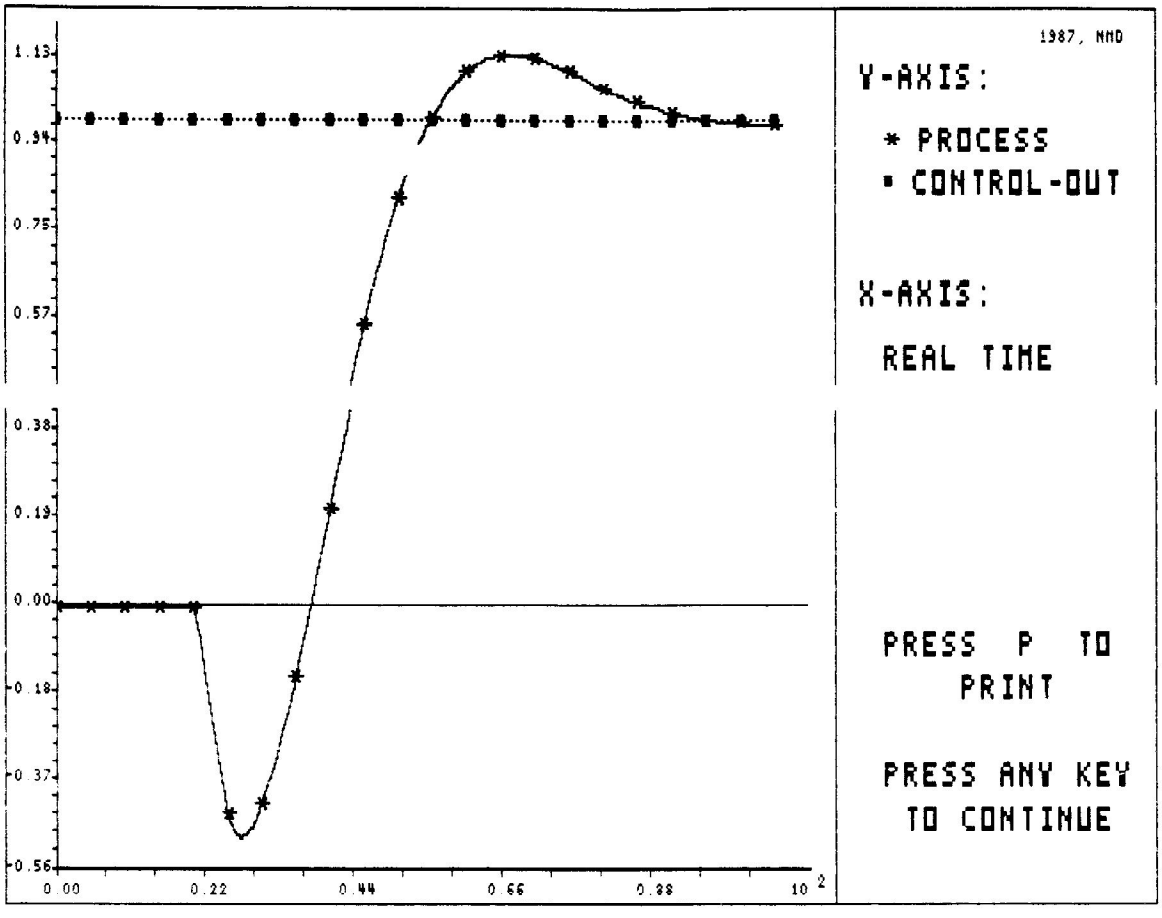
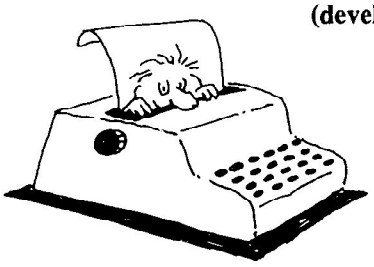



SUM OF ERROR SQUARED = 46.7687800
ENTER
1 - NEW SETPOINT/DISTURBANCE
2 - NEW TUNING PARAMETER
3 - NEW MODELING ERRORS
4 - NEW PROCESS
5 - EXIT

MICROCOMPUTER CHEMICAL ENGINEERING PROGRAMS

(developed by chemical engineering professors)



edited by Bruce A. Finlayson, University of Washington

Have you wondered what microcomputer programs are being used in other chemical engineering curricula? This column provides a mechanism for University professors to let others know about the programs they've developed and are willing to share on some basis.

The program should be described by a 250 word description, machine requirements, and ordering information. These programs should be ready to be shipped out the door, and should have been tested by students at more than one University. It would be helpful if the specific chemical engineering course were identified in which the program is useful. The programs will not be reviewed by Prof. Finlayson, nor will they be certified by CACHE.

In order to edit this column efficiently, submissions must be made to Finlayson via BITNET, using userid 27432 and node UWAV4. He will acknowledge receipt of the submission via BITNET, and will send the edited column to the CACHE office via BITNET. Letters will not be accepted. This requirement has two goals: to reduce the need for secretarial typing and to encourage academic chemical engineers to use electronic mail. You can find out how to use BITNET at your local installation—it is amazingly simple. You can then share the protocols with your colleagues for other uses.

This column can only be successful if you contribute. Let us hear from you!

Educational Software for Teaching Process Dynamics and Control

by Patrick Richard and Jules Thibault

DIRA (Didacticiel de Regulation Automatique) is a computer program written for the IBM PC to assist students in learning process dynamics and control. DIRA is menu-driven and efficiently uses the graphics capabilities of the IBM PC. Each option of the main menu corresponds to a particular topic covered in class. For continuous systems, the main options of DIRA include the inverse of the Laplace transform, the simulation of open- and closed-loop systems submitted to various types of input functions, the frequency response, the root locus and the identification of systems. For discrete systems, the main options are the inverse of the z transformation and the simulation of open- and closed-loop systems. The advantage of such a program is that students can rapidly change parameters of a particular simulation or calculation and readily visualize its effect, thereby enhancing their comprehension of the phenomena being studied. The last version is bilingual (French and English) and the language can easily be changed within the program.

To run the program, an IBM compatible with 384 kB of memory, a CGA card and one disk drive is needed. A disk with documentation may be obtained for $15 by writting to: Jules Thibault, Department of Chemical Engineering, Laval University, Sainte-Foy, Quebec, Canada, G1K 7P4.

MIDAS—Microcomputer Integrated Distillation Sequences

by Andrew Hrymak, McMaster University

This program was written by Ian Moore for a Masters project. It is based on the ideas of Andrecovich and Westerberg that the product of the heat load on the column and the temperature difference across the column is fairly constant over a reasonable pressure range. This idea can then be used as a guide in minimizing the energy consumption required for a separation over a

number of columns by sequencing the separations and integrating the column condensers and reboilers so that the full available process utility temperature range is used efficiently. Some of the complex column ideas of Hindmarsh and Townsend have been implemented. The columns are modelled using the shortcut techniques of Glinos and Malone.

The system thermodynamics is calculated with SRK. Heat loads and column sequences are shown graphically. The user need input only the critical property data, enthalpy data and binary interaction coefficients for the components of interest. MIDAS can write a file suitable for continued analysis with PROCESS.

The program is still being tested and should be considered in beta test stage. MIDAS has been written using Microsoft Fortran77 for IBM compatible machines and needs a CGA or EGA monitor. A coprocessor is strongly recommended. The source and executable code fit on two 360Kb diskettes. Changes to source require the purchase of the graphics library GRAFMATICS from Microcompatibles.

A test version may be obtained by sending a check for $10 to Andrew Hrymak, Department of Chemical Engineering, McMaster University Hamilton, Ontario, Canada L8S 4L7. A copy of Ian Moore's thesis can also be obtained to fully explain MIDAS and its use. You may also contact me via BITNET: HRYMAK at MCMASTER.

A Rigorous Multicomponent Multistage Steady-State Distillation Rating Program

by E.C. Roche, Jr.

Program DISTIL performs the rating evaluation of an existing multicomponent multistage distillation column. The program capabilities are 100 stages in the column (plus the condenser and the reboiler) and 9 components. The program can handle 6 feeds and 10 (vapor-liquid) side-streams/ intermediate heat exchangers.

Each stage in the column is considered to be a theoretical contact stage. The reboiler is treated as a kettle, while the condenser/reflux separator is considered a fractional equilibrium stage depending on the distillate product vapor/liquid split. The rating program assumes that the column geometry has been established, the operating pressure level is known, and that the feeds, side-stream withdrawals, and the intermediate heat exchangers are defined.

The available design variables are: (1) the distillate flow rate (vapor and liquid), (2) the reflux ratio or its equivalent (the boil-up ratio, condenser duty, and the reboiler duty), (3) the number of stages in the column, (4) the feed stage, and (5) the degree of feed vaporization. The solution of the nonlinear set of algebraic equations yields the stage compositions, flow rates and temperature. The solution method is the combination of the linear algebra method and the Newton-Raphson method.

The componential equilibrium and thermodynamic data is provided to the program in the form of tabular data. This form of data entry provides the student in a mass transfer course the opportunity to concentrate on what a rating program can accomplish.

The program was developed for a mass transfer course and has been in continued use for over fifteen years. The program is executable on IBM PCs using PC-DOS 2.0 or higher. The current version of the program requires an 8087 chip and 230K of available memory for the executable load module. The program interactively requests the input data file, and then generates a standard output file plus two additional files: a convergence trace file (also displayed on the screen) and a profile file of the converged case. The data in the profile file can be externally graphed to observe the column's operating characteristics.

A disk containing the program, documentation and illustrative examples may be purchased for $20, payable to Edward C. Roche, Jr. Send requests to E.C. Roche, Jr., 81 Brooklawn Drive, Morris Plains, NJ 07950.

RESIM: A Reactor Design Teaching Tool

by B.W. Wojciechowski

The Microsoft Fortran program RESIM is designed for the investigation of the cost and performance of isothermal and adiabatic reactors. It contains data files which at present allow the design of reactors using any of four methanol synthesis catalysts, one SO2 oxydation catalyst or

one ammonia synthesis catalyst. Other reactions and catalysts can be readily added as required.

The program has a wide range of design options which are entered in response to on-screen prompts. The numerical output is written to disk while graphical output can be sent to the screen or to an HP plotter. Pressure drop, Reynolds number in each bed, gas fugacities, heat exchange for cooling between beds, etc., are all included.

Finally, the program estimates the cost of the requested reactor design and specifies all reactor dimensions. The range of possible solutions for even one methanol synthesis catalyst is such that the program can be used to generate data for statistical experimental design studies.

The program is available in two versions: a version compiled on a Zenith 181 with 640K and an 8087 co-processor and a version compiled on an IBM mainframe, suitable for use on IBM PC terminals via Kermit. Both versions can be obtained in .EXE form by agreement from Dr. B.W. Wojciechowski, Chemical Engineering Department, Queen's University, Kingston, Ontario K7L 3N6, Canada.

Real-time Multiloop Computer Control Program, UC ONLINE

by Alan Foss

This program is designed for instruction in control system operation in undergraduate and graduate process control courses. Students can rapidly configure any imaginable multiloop control system for either laboratory apparatus or simulated processes. The program runs in real time and is interactive; changes can be made at any time.

Three types of PID controllers are available, each with a nonlinear gain feature, an auxiliary input for gain changes, and automatic status changes. Computational elements include summers, multipliers, dividers, square root, high and low selectors, A/D and D/A conversion, and lead-lags. Detailed and summary information about controllers and variables is displayed on separately accessed screens. Real- time graphical trend displays of any variable are available. The control configuration may be saved to disk and read in again.

Scores of on-line help files and some 50 pages of documentation and examples are provided. The program runs on IBM PCs and PS/2s and compatibles, 256K (512K recommended for use with simulations). A math coprocessor is necessary for extensive simulations. CGA, EGA, or VGA displays. Printer optional. Driver routines for Data Translation #2801 data acquisition board included.

Departmental license for any number of machines: $495.00. Address inquiries to Prof. Alan S. Foss, Department of Chemical Engineering, Gilman Hall, University of California, Berkeley, CA 94720.

Real-time Dynamic Distillation Simulation and Relative Gain Program

by Alan Foss

The distillation simulation is linked with our multiloop control program UC ONLINE, with which many different control systems may be configured and run.

The simulation models concentration dynamics only in a tray column separating a binary mixture. The user may select the relative volatility, number of trays, separation specifications, etc. as a means of setting the conditions of operation. "Measured" outputs of the simulation include top and bottom concentrations (delayed and error corrupted if desired), top and bottom temperatures, and column pressure drop. Five manipulatable inputs are the flow rates of the feed, reflux, distillate, boilup, and bottoms. The simulation is time-scaled to complete a transient in about 2 minutes. Included with the simulation is a preprogram for rapid specification of the column operating conditions and preparation of data files for use by the UC ONLINE control system. This program also calculates the relative gains for the column, quantities useful for deciding on the control system configuration.

This combination of programs is an effective tool for instruction in distillation control in process control courses. Runs on IBM PCs and PS/2s and compatibles, 512K and math coprocessor required. Simulation requires UC ONLINE multiloop control program. Departmental license for any number of machines: $200.00.

Address inquiries to Prof. Alan S. Foss, Department of Chemical Engineering, Gilman Hall, University of California, Berkeley, CA 94720.

The following programs have been listed in two prior editions of the CACHE News (Spring and Fall, 1987, Nos. 24 and 25). You can also obtain information about them from the conference "Chemical Engineering Software" on the Bulletin board GRAND@LSUCHE. To get started, send a Bitnet message:

To: Grand@LSUCHE

From: person id@node id

help

(1) Vapor Compression Refrigeration Cycle, by Stanley Sandler, University of Delaware.

(2) Compression of an Ideal Gas, by Stanley Sandler, University of Delaware.

(2) Computer-Aided Analysis for Process Systems, by Ted Cadman, University of Maryland.

(3) Discounted Cash Flow Analysis (and Present Worth), by Bruce A. Finlayson, University of Washington.

(4) Short-cut Distillation and Flash Calculations, by Bruce A. Finlayson, University of Washington.

(5) Convective Diffusion Equation (CDEQN), No. 25 and 26, by Bruce A. Finlayson, University of Washington.

(6) Engineering Plot (ENGNPLOT), No. 25 and 26, by Bruce A. Finlayson, University of Washington.

FLOWTRAN TAPES

_____I am interested in preparing a FLOWTRAN tape.

_____I am interested in obtaining a FLOWTRAN tape.

Please complete the following information. If you have two computers you would like to consider, duplicate this form and submit both completed forms and your preference.

1. Computer make and complete model number:

   _____

2. Operating system version:

   _____

3. FORTRAN compiler version:

   _____

4. Magnetic tape facility: No. of tracks _____ Drive speed in bits/inch _____

Name _____

Address _____

_____

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Please send this form to:

Prof. J. D. Seader
CACHE
3062 MEB
University of Utah
Salt Lake City, UT 84112

Please fill out this form only if you have not previously contacted Prof. Seader.

NEW OPTIMIZATION FEATURE FOR FLOWTRAN

by J. D. Seader

CACHE is pleased to announce to FLOWTRAN users the availability of a process optimization feature prepared by Prof. L. T. Biegler of Carnegie-Mellon University. With this feature, values of equipment parameters and feed-stream variables of process flowsheets can be optimized with respect to any user-written objective function.

This feature is made possible by three subroutines: SCOPT, OPT8 and QPSOL. SCOPT is an interface for connecting the FLOWTRAN simulator with optimization subroutines. OPT8 solves a nonlinear programming problem by successive quadratic programming (SQP). OPT8 calls QPSOL, a quadratic programming code, which has been licensed by Stanford University to CACHE for distribution to academic chemical engineering departments. SCOPT, which is used as a NEW BLOCK in the FLOWTRAN input data, is capable of infeasible-path, feasible-path and "black box" optimization. An important feature of SCOPT is that it permits simultaneous convergence of control and recycle loops, using Broyden's method, with the optimization.

Distribution of the optimization package is by means of FORTRAN 77 source code on a single 5 1/4" floppy disk for the IBM PC-DOS or MS-DOS operating system. Included on the disk are the subroutines:

SCOPT, 34,885 bytes
OPT8, 41,003 bytes
QPSOL, 164,140 bytes

These FORTRAN routines are easily added to FLOWTRAN by copying them into the FLOWTRAN program directory of your computer, compiling the routines to obtain object code, and adding that code to your FLOWTRAN object-library.

This optimization feature has been tested successfully on several problems of different complexity at four different sites, using three different major computer systems. Use of the feature is described in the new 3rd edition of *FLOWTRAN Simulation—An Introduction*, which includes a new chapter by Prof. Biegler on the optimization method. The method is also described by V-D Lang and Prof. Beigler in the article, "A Unified Algorithm for Flowsheet Optimization," in the journal *Computers and Chemical Engineering*, Vol. 11, No. 2, pp 143-158, 1987.

If you have previously obtained FLOWTRAN for your computer from CACHE and you have not already ordered the optimization package, please send a check for $50 US (for CACHE-sponsoring organizations) or $75 US (for those who do not sponsor CACHE) to:

CACHE Corporation
P.O. Box 7939
Austin, Texas 78713-7939

You will receive two copies of the "Stanford License Agreement" to sign and return so that you may use QPSOL. Upon receipt by CACHE of the signed forms, you will receive:

1. The FORTRAN 77 source code on a single 5 1/4" floppy disk for the IBM PC-DOS or MS-DOS operating system.
2. Instructions for installing the optimization routines into the FLOWTRAN program on your computer.
3. A copy of the new 3rd edition of *FLOWTRAN Simulation—An Introduction*, which describes how to use the new optimization feature.

STATUS OF FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

by J. D. Seader

As a part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to chemical engineering departments to install on their in-house computers. Thus departments would be able to run FLOWTRAN at no additional charge.

CACHE continues to supervise the preparation of FLOWTRAN load modules for some mainframe, supermini, and supermicro-type digital computers and the distribution of the modules on magnetic tape to departments that order them. A new optimization feature is now included, and the instructional FLOWTRAN book is now in its third edition. Please see the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

DEC VAX computers running with the VMX operating system.

DEC 20XX mainframe computer running with the FORTRAN-20 compiler (9-track, 1600 BPI tape).

UNIVAC 1100 series computers running under the EXEC 1100 operating system with the FORTRAN compiler (9-track, 1600 BPI tape).

Amdahl computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).

IBM and IBM-plug-compatible mainframe computers such as the 370, 30XX and 43XX with the following operating system and FORTRAN compiler combinations:

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	OS1/MVS	IV-H ext.
c	OS/VS2 MVS	VS
d	CMS	IV-G1

IBM PC-XT 370 PC operating in conjunction with an IBM mainframe.

CDC Cyber mainframe computers with the NOS operating system and a FORTRAN V compiler.

Apollo Domain workstations running with AEGIS operating system (program on floppy disk).

Data General MV superminicomputers running with the AOS/VS operating system.

Honeywell computers with CP6 operating system.

Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes but not for consulting. 156 FLOWTRAN tapes and floppy disks have already been distributed.

If you would like to obtain a FLOWTRAN tape for your computer and have not already contacted CACHE, complete and submit the FLOWTRAN TAPE form at the end of this newsletter. You will be required to sign a User's Agreement that must be approved by Monsanto. The cost of the tape, payable to CACHE, is $250. The charge to CACHE-supporting departments is $175.

MATHEMATICAL SOFTWARE AVAILABLE FROM LEHIGH UNIVERSITY

Lehigh University has prepared mathematical software with many chemical engineering applications. The following descriptions were provided by William E. Schiesser in the chemical engineering department. All software is available to both educators and industry. Academic institutions are eligible for a substantial discount. Please address inquiries to:

W. E. Schiesser
Mountaintop Campus
Building A (111), Room D307
Lehigh University
Bethlehem, Pennsylvania 18015 USA

He can be reached by phone at (215) 758-4264 or (215) 758-5486. Dr. Schiesser's BITNET address is WES1@LEHIGH.

DSS/2, Release 4

DSS/2 is a widely distributed computer code for the numerical solution of systems of algebraic, ordinary and partial differential equations (AE, ODE and PDEs).

Release 4 includes new features: routines for the direct calculation of second-order spatial derivatives in second-order PDEs, adaptive gridding for one-dimensional PDEs and orthogonal collocation on finite elements in one, two and three dimensional spatial domains.

All of the coding is in transportable FORTRAN 77 and will execute on any mainframe or minicomputer with a FORTRAN 77 compiler, e.g., IBM series 43XX, 9370, 30XX, DEC VAX and MicroVAX, CDC Cyber. All of the features of earlier DSS/2 releases have been retained in Release 4 and all applications running under earlier releases will run without modification under Release 4.

The DSS/2 package includes: (1) two none-track tapes with the DSS/2 FORTRAN source code in single and double precision formats plus all of the problems in the seven manuals, (2) the output from ten test problems for checking the operation of the code and (3) a set of seven manuals.

Sets of applications are available separately in physics, chemistry, applied mathematics, fluid flow, heat transfer, mass transfer and separations, kinetics and chemical reactors, process control, and biochemical, biomedical and environmental systems. Each set consists of documented FORTRAN subroutines called by DSS/2 and contains about 40 titles.

Micro-DSS

This is a version of DSS/2 written for the IBM AT with color graphics. It is available on a 1.2 megabyte diskette.

ODE Pack

ODEPACK is a set of six quality integrators developed by Dr. A. C. Hindmarsh of the Lawrence Livermore National Laboratory for the numerical solution of systems of algebraic and initial-value ordinary differential equations. The six integrators can be applied to the following specific problems:

LSODE: (Livermore Solver for Ordinary Differential Equations): The basic solver for systems of ODEs, i.e., dy/dt+f(t,y) with full or banded processing of the Jacobian matrix of f(t,y).

LSODI: A solver for systems of ODEs defined in a linearly implicit manner, i.e., **A** *dy/dt=f(t,y) where **A** =A(t,y) is a square matrix. ODEs of this form typically arise in finite element and weighted residual applications.

LSODA: A variant of LSODE with automatic selection of stiff or nonstiff options as the solution proceeds; the user need not be concerned with the issue of stiffness.

LSODAR: A variant of LSODE and LSODA which additionally finds roots of given functions of the solution vector.

LSODES: A variant of LSODE which treats the ODE Jacobian matrix in general sparse matrix form; for the stiff options, the linear systems are solved by the Yale Sparse Matrix Package (YSMP).

LSOIBT: A variant of LSODI designed specifically for block-tridiagonal matrices.

DASSL

A quality integrator for differential-algebraic systems developed at the Lawrence Livermore National Laboratory.

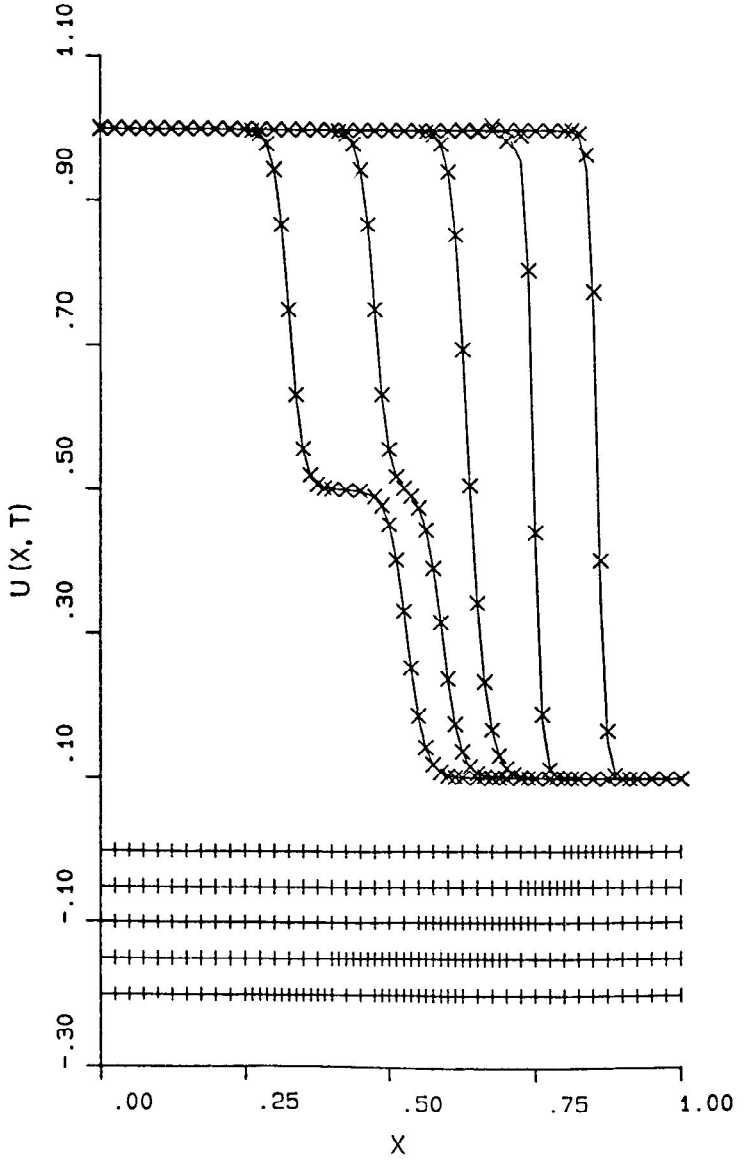
HOMPACK

A library of routines for the solution of systems of nonlinear equations by globally convergent homotopy algorithms.

GRD1

A code for the numerical integration of stiff and nonstiff ordinary differential equations and one-dimensional partial differential equations on an adaptive grid.

Adaptive Grid Solution of Burgers' Equation



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Prof. Brice Carnahan
Chemical Engineering Dept.
The University of Michigan
Ann Arbor, MI 48109

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signed date

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institution _____
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Basic Package

$ 400. _____

Software:

1. MicroCACHE Module Presentation (**MSM**) Diskette
2. MicroCACHE Module Preparation/Information Retrieval (**MCU**) Diskette
3. MicroCACHE McCabe-Thiele **MOD**ule (MCCABE) Diskette
4. MicroCACHE McCabe-Thiele Module **Source** File Diskette

Documentation:

1. *Overview*
2. *User's Manual*
3. *Instructor's Manual*
4. *Module Writer's Manual*
5. *Graphics Packages Manual*

Videotapes (VHS Format):

1. *The MicroCACHE CAI System*
2. *Module Preparation I*
3. *Module Preparation II*

Modules

1.	a) Interactive Graphical Flowsheet Preparation b) Steady-State Process Simulator (Mat. Bal. Only) (CLASS)	$ 150. _____
2.	Material Balance Exercises (MATBAL)	$ 90. _____
3.	Binary Distillation - Ponchon-Savarit Method (PONCH)	$ 90. _____
4.	Binary Batch Distillation (BATCH)	$ 90. _____
5.	Solution of Single Nonlinear Equations* (NLEQN)	$ 90. _____
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7.	Solution of Systems of Linear Equations (SLINEQ)	$ 90. _____
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10.	Linear Programming (LINPRO)	$ 90. _____
11.	Nonlinear Programming (Dav.-Fletch.-Powl./Broyd)* (UNLP2)	$ 90. _____
12.	Gas Reservoir Simulation (GASSIM)	$ 90. _____

TOTAL _____

*Module requires that a copy of the MicroSoft FORTRAN-77 compiler be available. These modules should be used only on PCs with hard disks (e.g., XT,AT).

Please **sign** the reproduction/distribution **agreement** on the reverse side, **enclose purchase order** or **check** (payable to CACHE) for total amount, and return to Prof. Carnahan.

FLOWTRAN BOOKS

send to: ULRICH'S BOOKSTORE
Attn: Heather Senior
549 E. University Avenue
Ann Arbor, MI 48109

Please send me:

Flowtran Simulation—An Introduction, 3rd edition; by J. D. Seader, W. D. Seider & A. C. Pauls.

No. of copies_____@$16.95/copy

Add $1.50 per copy for mailing and handling in the U.S. A check must accompany all orders by individuals. Also available in quantity at regular quantity discounts to established book retailers.

Name _____

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Make checks payable to Ulrich's Bookstore.

CACHE PROCESS DESIGN CASE STUDIES

All case studies are $35 including postage (book rate in the U.S. and surface mail for orders shipped overseas). The initial copy for departments that support CACHE is $15.

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WHAT IS CACHE?

CACHE is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960s the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, fourteen chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. The CACHE Committee was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers including both educators and industrial members and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its ongoing projects. Information on CACHE activities is regularly disseminated through **CACHE NEWS**, published twice yearly. Individual inquiries should be addressed to:

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CACHE NEWS

The CACHE News is published twice a year and reports news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by D. M. Himmelblau with contributions from a number of CACHE members and representatives.

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