CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 32 Spring 1991

The CACHE CORPORATION

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 editied by D. M. Himmelblau with contributions from a number of CACHE members and representatives.

CACHE NEWS

No. 32 Spring 1991

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TANKSPILL - A Process Control Game

by Sigurd Skogestad and Erik Wolff
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This game, run under Microsoft Windows, simulates a tank with a gas and liquid feed, and the objective is to keep the pressure and liquid level in the tank at given values by manipulating the valves of the streams leaving the tank. The parameter values chosen in this game are intended to represent a gas-oil separator where a high-pressure well stream is separated into liquid and gas. Condensation or vaporization is neglected. The objective of the game is to introduce the student to the dynamics of an interacting process.

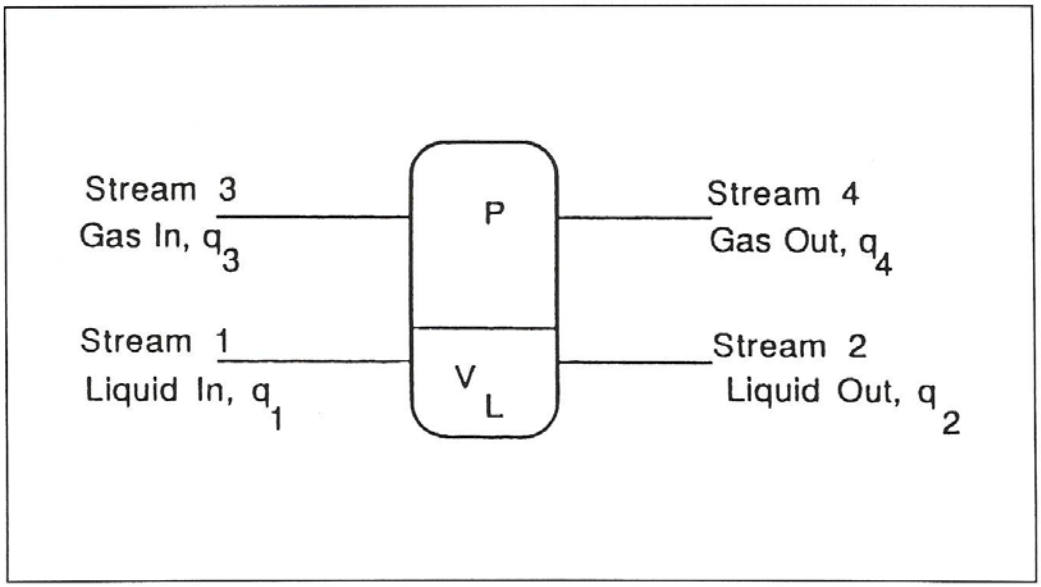
The program may be run with or without a predefined set of disturbances, and the valves may be operated manually (with a mouse) or with a P-, PI- or PID- controller. The program may be used to illustrate various aspects of process control ranging from an introduction to dynamics to controller tuning.

In Training mode the disturbances may be changed by the user. In this way a student can use step responses etc. to tune his/her own controller.

In game mode the objective is to maximize the game time. The student starts with 1000 points and points are subtracted if the level and pressure deviates from their setpoints.

'TANKSPILL' operates under WINDOWS, and a AT, PS/2 or compatible with a 286 or 386 processor is needed for acceptable speed. A color monitor is neede to identify streams etc. It is possible to operate the program with a keyboard only, but the use of a mouse is recommended.

Model of the System



The system has four independent variables (flows). The manipulated variables (inputs) are Z_2 and Z_4, the valve opening on the streams leaving the tank. Disturbances are q_1 and q_3 the flowsof the streams entering the tank. The system is described by the following differential equations:

Material Balances

$$dV_L/dt = q_1 - q_2 \qquad [m^3/s]$$

$$(V - V_L) * dP/dT = RT*(q_3 - q_4) + P*(q_1 - q_2) \qquad [Pa*m^3/s]$$

Valve Equations

$$q_2 = Cv_2 * f(z_2) * (P_L - P_{LO})^{1/2} \qquad [m^3/s]$$

$$q_4 = Cv_4 * f(z_4) * (P^2 - P_{GO}{}^2)^{1/2} \qquad [kmol/s]$$

Linear valves $f(z_1) = z_1$, where $z_1 = [0,1]$

$$P_L = P + gV_L/A$$

Nominal Steady-state Operating Conditions

$V_L = 20\ m^3$

$P = 70$ bar; $P_L = 70.07$ bar; $P_{Lo} = P_{Go} = 60$ bar

$z_1 = z_2 = 0.5$

$q_1 = q_1 = 4.0\ m^3/s$

$q_2 = q_2 = 2.56$ kmol/ s

$T = 400$ K

Constraints

$0 < V_L < 100\ m^3$; $P < 100$ bar

There is a 5 second dead-time in the valve- dynamics which is modelled using a 5th order lag. In terms of Leplace transforms:

$$dz_2 = 1/(1+s)^5 * dB/100$$

$$dz_4 = 1/(1+s)^5 * dD/100$$

where z_2 and z_4 are the actual valve openings, and D and B are the desired valve openings (in %) set manually or by the controller.

Linearizing the model at this steady state yields:

$$\begin{pmatrix} dV_L \\ dP \end{pmatrix} = G(s) \begin{pmatrix} dB \\ dD \end{pmatrix}$$

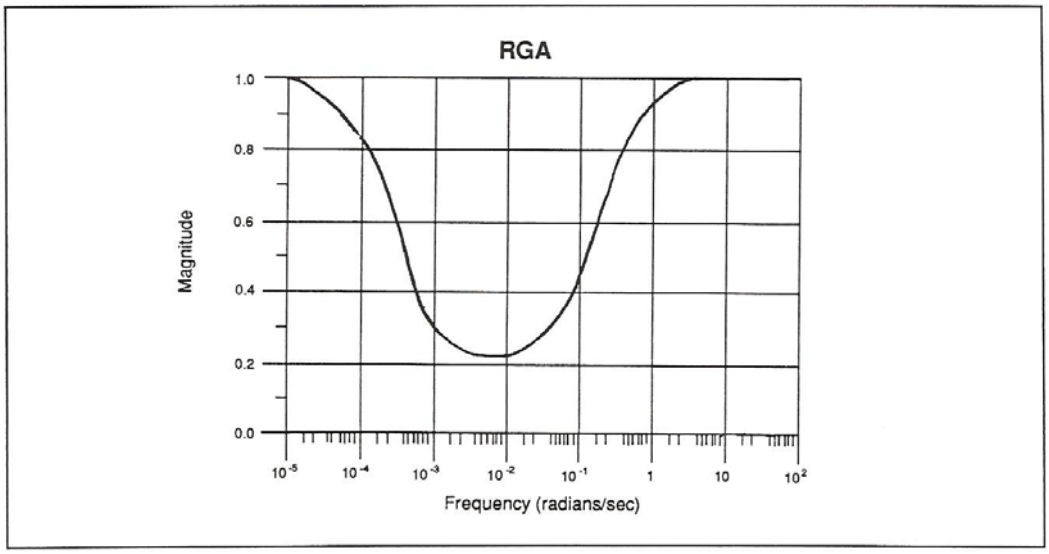
where B and D are the valve openings in percent.

Here:

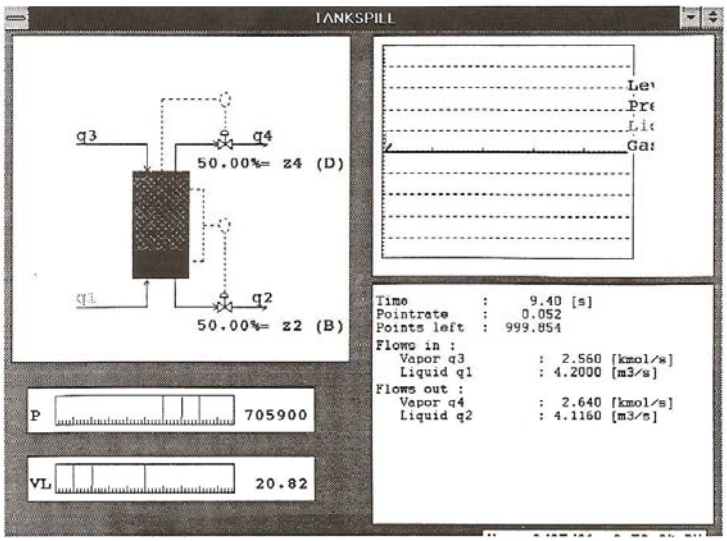
$$G(s) = Gc(s) * 1/(1+s)^5$$

$$Gc(s) = \frac{0.01}{(s + 1.72e^{-4})(4.32 * s+1)} * \begin{bmatrix} -34.54*(s+0.0572) & 1.913 \\ -30.22e+5 * s & -9.188e+5*(s+6.95e-4) \end{bmatrix}$$

The small eigenvalue of $-1.7e^{-4}$ comes from the self-regulation of liquid level which is almost negligible. As noted above the process is very interactive. The RGA has a steady-state value of 1 (see figure on succeeding page), then goes down to 0.25 at a frequency of 0.01 Hz, and returns back to 1 at about 1 Hz. This implies that interactions increase the effective gains of the loops and that interactions are most severe at intermediate frequencies. The system is triangular (and therefore has a RGA-value of 1) at steady-state because liquid flow has no effect on pressure at steady state, and the system is triangular at high frequency because the gas stream has a direct effect on pressure, but only an indirect effect on level. Note that the interactions will be more severe if the controllers are detuned than when they are tightly tuned. The interactions make this a challenge problem for single-loop control and introduces the students to some important aspects of multivariable control.



Screen Display



Use of TANKSPILL for Teaching

In our process control course, which is currently based on the book by Stephanopolous we have about five exercises where the game is used. It is a good idea to use one lecture to introduce the students to the problem.

1. After 1-2 weeks of teaching the students have an exercise divided into three parts:

   A) Find the mathematical model for the tank.

   B) Use "training mode" to perform steps in flows q1, q2, q3 and q4.

   C) Use "game mode" to achieve maximum game time with manual control and with P-control. The students will discover that it is much easier to get good response with P-control.

2. Two weeks later the students are asked to simulate the same process using MATLAB, but without the lags on the inputs. They are asked to compare the simulations they did with TANKSPILL. It is important to note that in TANKSPILL you change the valve position, and only indirectly the flow. For example, you will see in increase TANKSPILL that increasing z4 (ie., D) will first yield an increase in q4, but q4 will eventually return to its original value. On the other hand, it should be noted that changing z1 and z3 directly changes the inlet flows.

3. The next week they are asked to linearize the model equations analytically and obtain numerical values for the coefficients at the nominal steady state.

4. Finally, about 3 weeks later they are asked to:

   A) Based on the linearized model, obtain the transfer matrix GC(s).

   B) Use training mode with P-control to obtain Ziegler-Nichols PID tunings. Use these in game mode with PID control.

5. At the end of the course the TANKSPILL example is used to illustrate that the steady-state RGA may be misleading in some cases. At steady-state the RGA-value is 1. However, we know that there are dynamic interactions in TANKSPILL, and these are illustrated by plotting the frequency-dependent RGA.

If interested in a free copy of TANKSPILL, please complete the Standard Order Form in the back of the Newsletter and return to CACHE Corporation.

NSF Electronic Proposal Submission Project: A Report

By Peter Rony, Virginia Tech

The following information was received by the CACHE Electronic Communications Task Force in August 1990. In addition to the announcement of the project, which is being published in this issue of CACHE News, there are two companion documents that need to be acquired by an interested university: (1) PS-EXPRES Users' Guide, Version 2.1.2 (July 26, 1989), and (2) PS-EXPRES Version 2.1.2 Annoucement (February 9, 1990). Electronic versions of all three documents can be obtained either by:

(a) accessing the file server,
chelib@emx.utexas.edu
(details for accessing this new file server are give elsewhere in this newsletter)

(b) sending a request to
rony@vtvm1

(c) accessing the file server,
grand@lsuche

For a written copy of the documents, please write to:

Dr. Gerald B. Stuck
Director, Electronic Proposal Submission
National Science Foundation
1800 G St. NW, Room 401
Washington, DC 20550
<gstuck@nsf.gov> (Internet)

Goal

The Electronic Proposal Submission (EPS) Project is intended to begin the process of changing the way NSF receives and processes proposals. The Foundation goal is to enable and encourage electronic proposal submission. In order for this process to become routine, there is much to learn at universities and NSF. This project is being undertaken so that we may begin this learning process.

Background

EXPRES (EXPerimental Research in Electronic Submission) is an NSF funded research and development project to create a specification, in the form of a prototype, of a next generation information technology environment to support NSF and its scientific/engineering constituency in the creation, submission, and review of research proposals. One of the critical elements in the EXPRES activity is impact on NSF. As part of the ongoing discussions of integrating new technology into NSF (especially the proposal process) there have been recommendations regarding relatively low-cost interim experiments involving electronic proposal transmission and review. NSF's Office of Information Systems (OIS) and the EXPRES program office (CISE) have cooperated in defining several of these experiments.

Approach

The primary concern of this project has been to define an approach which can be utilized in a number of technological environments. Our approach has been to utilize industry standards for the electronic proposal. An NSF proposal contains data (proposal forms) and proposal text (intellectual content). The data is transferred to NSF central data bases for proposal processing. NSF has defined a file format for the data elements associated with the proposal forms. This file is in ASCII format and utilizes a field name/value pair approach. Each line in the file contains a field name and a value. Since this file is in ASCII format, it can be created in a number of software/hardware environments. The second part of the proposal is the proposal text including graphics. Many proposals are created by text processors which can output high quality text and graphics. Most of the output is generated on PostScript (a trademark of Adobe Systems, Inc.) compatible laser printers. Since PostScript is device independent, it was chosen as a standard for receipt of proposal text.

Carnegie-Mellon University, as part of the EXPRES grant, has prepared a set of PostScript-based proposal generation

tools (PS-EXPRESS) from which one can prepare a proposal to be submitted electronically to NSF. The proposal cover sheet and other NSF forms are prepared from an ASCII data file in the NSF-specified format. The PS-EXPRES software attaches the ASCII file to the PostScript proposal. This proposal file can then be transmitted electronically to NSF for processing.

Electronic Proposal Submission Participation

The following are the requirements for participation in the electronic proposal submission project:

1. Designate a contact point at your institution from which proposals will be transmitted to NSF. This contact point must have an e-mail address and have access to the TCP/IP file transfer protocol (ftp) software for transmission of proposals to NSF. Your proposals will be transmitted from the single institution contact to a single NSF office. A typical contact would be a research administration office with some computer support expertise.

2. The institution must have the capability to produce the proposal in PostScript output form. Many text processing software packages can produce PostScript output. The PS-EXPRES software provides the capability to create the NSF forms and combine them with the proposal body. The institution should also have access to a PostScript laser printer in order to print copies for their own use.

3. Use the PS-EXPRES software which is distributed without cost by NSF and Carnegie Mellon University (see Attachment). The proposal cover sheet and other NSF forms are prepared from an ASCII data file in the NSF-specified format. The PS-EXPRES software attaches the ASCII file to the PostScript proposal. This proposal file can then be transmitted electronically to NSF for processing.

4. Deadlines. Paper proposals are deemed received when delivered to the NSF proposal receipt area. The electronic date stamp on the NSF receiving host will determine receipt for proposal deadlines under this project.

5. Program Assignment. All proposals received during this project will be addressed directly to an NSF division and if possible a particular program and program contact. This will assist OIS in making the proper proposal assignment and ensure that the subsequent signed proposal copy will be forwarded to the proper office.

6. Authentication. The current procedure is for the institution to send a single signed copy after receipt and logging at NSF of the electronic copy. This procedure may change in the future.

Processing Procedures

The following processing procedures will be used for the EPS Project:

1. Request participation in this project by sending mail to <nsfprops@nsf.gov> designating an institution point of contact.

2. In order to submit a proposal, send mail to <nsfprops@nsf.gov> stating that you intend to send an electronic proposal and requesting instructions. You will receive a message indicating the user account and password for transferring the proposal file to NSF. Following is a sample session:

Sending Electronic Proposals to NSF:

Use FTP to transfer the proposal to a machine at NSF. Following is the process for transferring the file. You may substitute a name of your choice for "yourproposal" in the following process:

```
>ftp 128.150.195.43 <n1.nsf.gov>
ftp> Name: submit01
ftp> Password: password
ftp> put yourproposal
ftp> quit
```

3. Once the transfer succeeds, send mail to <nsfprops@nsf.gov> as notification. NSF will file the proposal and delete it from the above user account. An e-mail notification will be sent back to you. After receiving the e-mail acknowledgment, send a single signed copy to NSF as authentication.

4. Additional copies for NSF programs will be handled internally by NSF.

Dynamic Simulation Using TUTSIM and OrCAD [1]

By Peter R. Rony, Virginia Tech

TUTSIM Block-Diagram Simulation Language [2]

TUTSIM, an acronym for Twente University of Technology SIMulation program, is a high-level, block-diagram language that basically functions as an analog-computer-on-a-PC. Engineers from the late 1950s through early 1970s may recall that an analog computer was usually programmed from a block diagram sketch and a list of equations representing the system to be modeled; the analog computer solved the problem by substituting functional, analog-electronic hardware circuits (based upon operational amplifiers) for real functions.

TUTSIM re-establishes the analogy between real-world systems and a computer modeling language. Ninety-three defined blocks from SUM, GAIn, MULtiply, DIVide, and INTegrate through X,Y FuNCtion, Laplace functions, logic blocks, Z-transform blocks, and thermodynamic property blocks combine the convenience of the analog computer with the accuracy and speed of personal computers, specially those that employ an arithmetic coprocessor chip (8087, 80287, 80387). A very valuable block is the SYC (synchronization) block, which synchronizes the TUTSIM simulation time base to the real-time clock within the personal computer. During a simulation, the output of SYC can be monitored to determine how well the synchronization is proceeding.

The wide variety of TUTSIM blocks allow a user to describe virtually any physically-reasonable mechanical control, process control, or differential equation, continuous or discrete. Of considerable importance, non-linear differential equations are generally no more difficult to model than linear differential equations.

Special features of TUTSIM that make it valuable in an educational environment include: (a) tabular or graphical output, either printed or as an electronic file (graphical screens can be captured); (b) toggle of 80n87 arithmetic coprocessor to speed program execution; (c) up to four simultaneous plots per graph; (d) multi-run capability, which permits the overlay of graphical plots for a sequentially incremented process variable; (e) macro commands such as save macro, import macro, list macro, and concatenation of model files; (f) ability to important tabular data (parameter pairs) from an ASCII file; (g) ability to write simulation results in IEEE Long Real Floating-Point format to a disk file, which can be read by PC-MATLAB as well as most programs written in the C language; (h) direct search parameter estimation facility, an implementation of the SIMPLEX method by Neader and Mead; (i) selection of a variety of CRT displays, for example, CGA, Hercules, and EGA; (j) real-time I/O through the use of customized, assembly-language object code for input/output boards that fit into the IBM-class backplane; (k) user-defined blocks written in either C, FORTRAN, or PASCAL; (l) input of arbitrary, piecewise-linear function data; (m) thermodynamic-property blocks; and (n) creation of TUTSIM block diagrams using the OrCAD/SDT III schematic design tool.

Academic licenses and student products are available upon request [2]; student versions that are restricted to 27 blocks, including manual, cost $30-$35. "Personal TUTSIM," a full-sized, full- featured package with all the power and capabilities of the commercial $695 version is marketed for a price of $139.50; it is sold only for the personal use of the buyer, and not for any corporate, government, or classroom use.

OrCAD Computer-Aided-Design (CAD) Software [2]

OrCAD/SDT III is an electronic design automation tool that is widely used for the capture of electrical schematic designs. In its common application, OrCAD/SDT III comes with 6200 unique library parts in over 40 integrated-circuit libraries. Structured design features within OrCAD/SDT III provide a hierarchical approach to organizing designs that contain up to 4000 sheets through the strategy of partitioning the design into smaller, more manageable sections. Over 200 hierarchical levels simplify complex tasks. With over 30,000 packages sold, OrCAD is the de facto industry standard for easy-to-use schematic capture.

TUTSIM Products markets, for $149, TUTSIM/OrCAD interface software that permits the creation of hierarchical TUTSIM block diagrams and simulation models for direct input into TUTSIM using OrCAD/SDT III, which is independently marketed (call TUTSIM for a price quote). The TUTSIM/OrCAD interface includes a complete block library of all individual TUTSIM blocks, an OrCAD-to-TUTSIM conversion program, and a TUTSIM-to-OrCAD conversion program for parameter changes and plotblock scaling. Several OrCAD diagrams will be illustrated in this article.

TUTSIM User-Defined Block Option [1, 2]

Tutsim Products markets special software, the "User-Defined Block Option," that provides almost unlimited extensibility to the block-diagram functions of TUTSIM. This "Option" allows a user to create a new type of TUTSIM block—USA/USR—that may add functions such as memory access to I/O hardware boards or, alternatively, may act as windows and linkages to complex code sections that are not limited to simple math functions. With USA/USR blocks, different displays, recording devices, or I/O devices may be addressed and incorporated into the TUTSIM model simulation.

To create a new TUTSIM block diagram function, a user completes a C or FORTRAN source-code skeleton that is then compiled into a file, USRBLK.EXE, that executes in parallel with the main TUTSIM executable file TUTEXEC.EXE on an IBM-class personal computer, preferably one equipped with a math coprocessor.

BLENDER1.SIM OrCAD/TUTSIM Simulation Program [1]

Consider the blender unit of a three-component blender/packaging process. As illustrated in Figure 1, water (H2O), an aqueous suspension of component A, and a dilute aqueous polyelectrolyte suspension agent B are added to the blender tank, where they are mixed and heated. The solution is cooled and then transferred to a packaging unit (not shown in the figure). Under the assumptions that the jacket and the reactor are both perfectly mixed, the volume of the jacket and all physical properties are constant, the densities and heat capacities of all inlet and outlet streams are approximately the same, and heat losses are absent, the model equations are given in Figure 2.

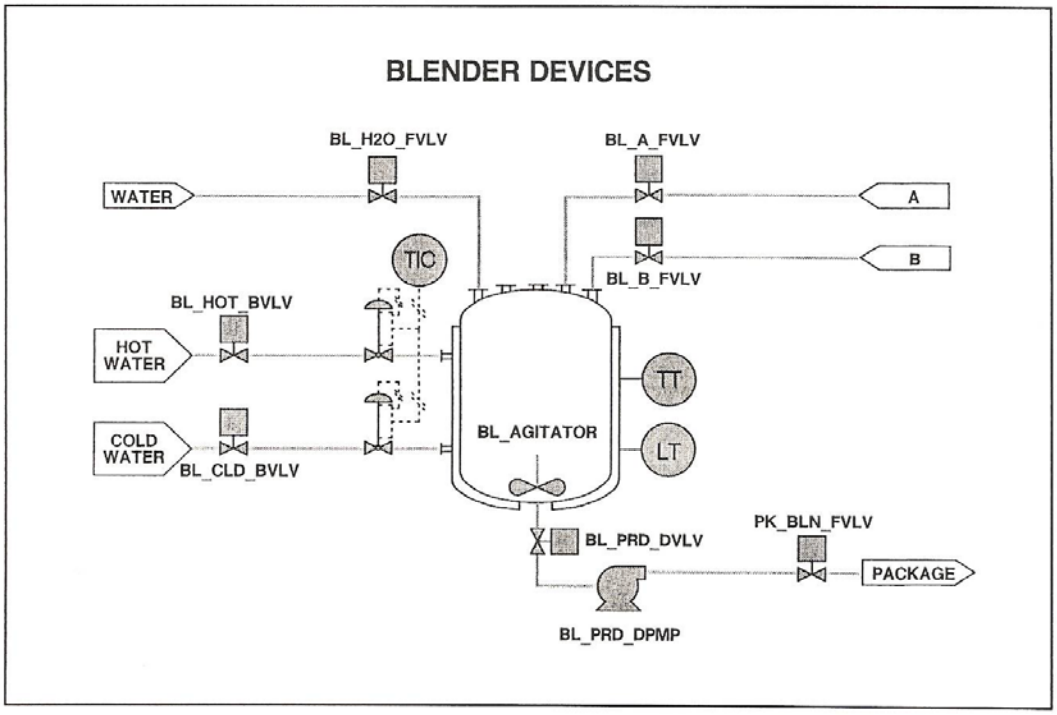


Figure 1.

The BLENDER unit in the three-component, blender/packaging process. Device names are specified.

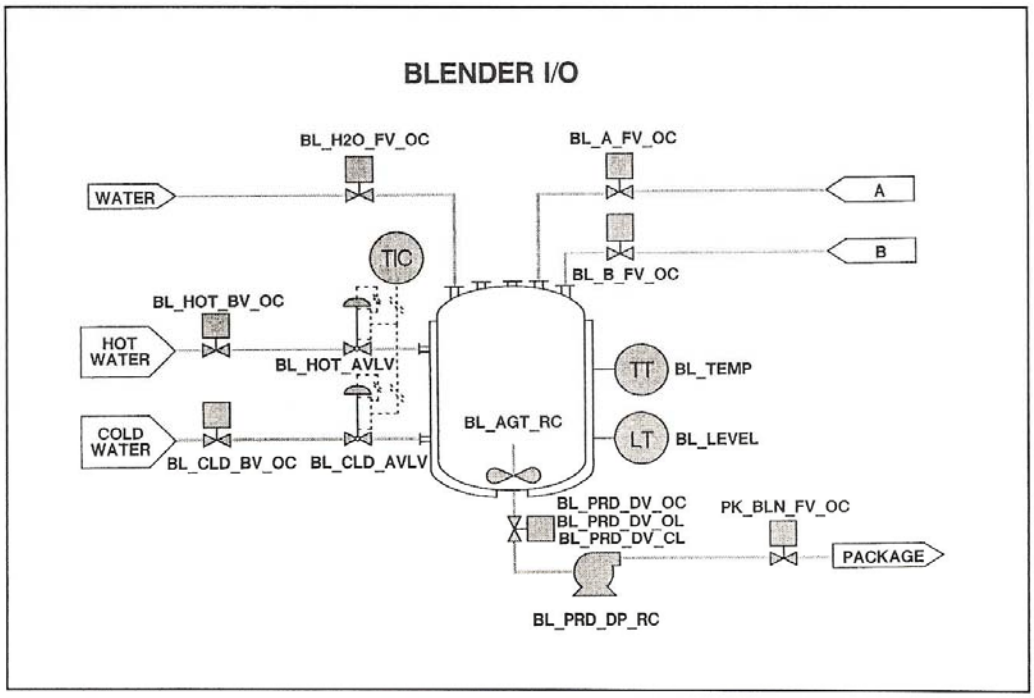


Figure 2.

The BLENDER unit of Figure 1 with blender I/O signal names specified.

A similar process example, a continuous stirred-tank reactor simulation, is discussed in Chapter 9 of Smith and Corripio [3]; this well-documented example was used by these authors to demonstrate different approaches to the computer simulation of dynamic process models. Our article adds yet another approach (TUTSIM) to controls process simulation, one that we believe is both simpler and more intuitive. Further, this approach now lends itself readily to the development of testable control design software when a Texas Instruments TI 500 Series controller and APT software are used concurrently [1].

The blender I/O variables are defined in Figure 3. The BL_***_OC variables are block-valve open commands for the inlet, outlet, hot, and cold fluid streams; BL_TEMP and BL_LEVEL are transmitter variables.

Equations (1) through (3) in Figure 2 were simulated by a TUTSIM model, called BLENDER1.SIM, that contained 62

CAD software was used to create and document the TUTSIM block- diagram simulation model for the blender. OrCAD/SDT III was applied to the task of simulating the system, including the exchange of values of twelve variables,

BL_LEVEL.RAW, BL_TEMP.RAW,
BL_CLD_BV_OC, BL_HOT_BV_OC,
BL_CLD_AVLV, BL_HOT_AVLV,
BL_PRD_DV_OC, BL_PRD_DP_OC,
PK_BLN_FV_OC, BL_H2O_FV_OC,
BL_A_FV_OC, and BL_B_FV_OC

that were common both to the BLENDER1.SIM program and a corresponding APT program, DEMO_01E, running in the TI 500 Series controller[1]. BL_LEVEL.RAW, BL_TEMP.RAW, BL_HOT_AVLV, and BL_CLD_AVLV are 16-bit controller input variables; the remainder are Boolean controller output variables.

$$dV/dt = F_{H2O} + F_A + F_B - F \quad (1)$$

$$dVT/dt = (F_{H2O} + F_A + F_B) T_i - FT - UA \ (T-T_j)/\rho C_p \quad (2)$$

$$dV_j T_j/dt = U_j A_j (T-T_j)/\rho_j C_{pj} - F_j (T_j-T_{ji}) \quad (3)$$

where

V is the blender volume, m^3

V_j is the jacket volume, m^3

T is the blender temperature, C

T_j is the jacket temperature, C

T_{ji} is the inlet jacket temperature, C

T_i is the inlet temperature of water, solution A, and solution B, C

F_{H2O} is the inlet water flow rate, m^3/s

F_A is the inlet aqueous solution A flow rate, m^3/s

F_B is the inlet aqueous solution B flow rate, m^3/s

F is the outlet flow rate, m^3/s

F_j is the jacket flow rate, m^3/s

ρC_p is the product of the density and heat capacity of the blender inlet and outlet flow streams, $J/m^3 C$

$\rho_j C_{pj}$ is the product of the density and heat capacity of the jacket flow stream, $J/m^3 C$

UA is the product of the blender tank heat-transfer coefficient and heat exchanger surface area, $J/s-C$

$U_j A_j$ is the product of the jacket tank heat-transfer coefficient and heat exchanger surface area, $J/s-C$

Figure 3

The three non-steady state equations, along with variable and parameter definitions, for the blender in Figure 1.

Figures 4 through 8 illustrate the hierarchical, OrCAD approach to the generation of the BLENDER1.SIM simulation model for the system in Figures 1 and 3. Figure 4 represents the highest level of the hierarchy, which includes schematic blocks for the non-steady-state total mass balance (top block, Eq.1); the non-steady-state energy balance for the blender tank (third block, Eq. 2); the non-steady-state energy balance for the jacket (fourth block, Eq. 3); and the calculation of blender flow information (second block). The ten USR blocks in Figure 8, each associated with a block or analog valve, can be understood with the help of Figure 3.

The unusual feature that distinguishes Figures 4 through 8 from a traditional process simulation in a high-level language is the USR block, specially those in Figure 8. Not only have the transient mass and energy balances been solved, the behavior of the valves and pump in the model have also been incorporated. The flows of H2O, A, B, cold water, or hot water do not occur unless the respective valve receives an open command from the TI 500 Series controller software. This may seem to be a small accomplishment, but it becomes important when the batch process control strategy incorporates automatic sequencing, which determine the timing of the valve behavior. All of the I/O points can be simulated in the TUTSIM model, and the testing of the controller strategy can be relatively complete. Nine-hundred ninety-nine (999) TUTSIM blocks are sufficient to simulate an entire midrange process.

A reader who is familiar with the TUTSIM block diagram language would observe two recognizable features of the language in the OrCAD Figures 5 through 8: (1) all values of the block parameters are provided below the lower-left-hand corner of each block, (2) a comment can be provided above each block.

The use of OrCAD increases the time associated with the creation of a TUTSIM model, but offers the academic and industrial advantages of more effective process model documentation, communication, and maintenance. In an academic environment, the cost of OrCAD/SDT III is prohibitive for an individual student; unfortunately, an attractively priced, restricted, student version tailored specifically to the TUTSIM block diagram language does not exist.

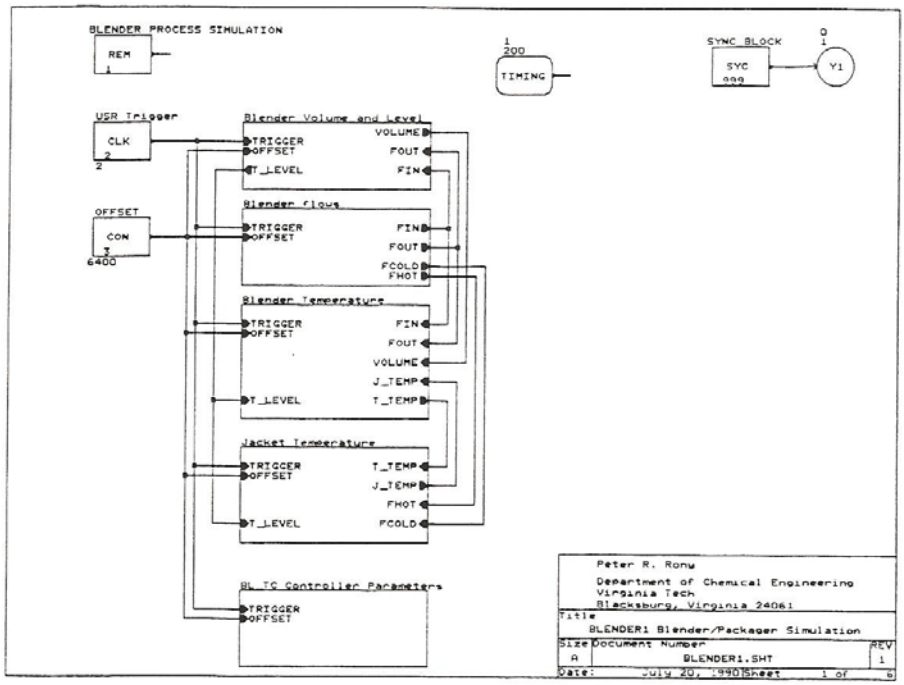


Figure 4

The highest level of the OrCAD hierarchy for the disign of the TUTSIM blender simulation: overall schematic for the BLENDER 1.SIM blender simulation.

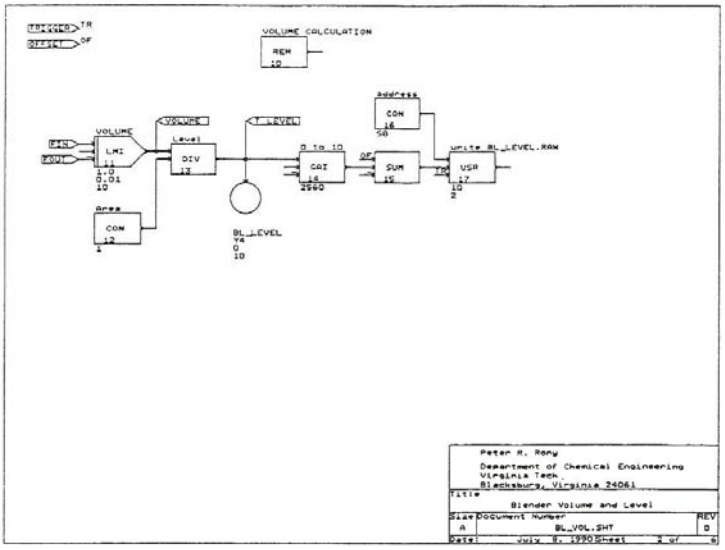


Figure 5

The TUTSIM/OrCAD diagram that represents the non-steady state equation for the blender volume.

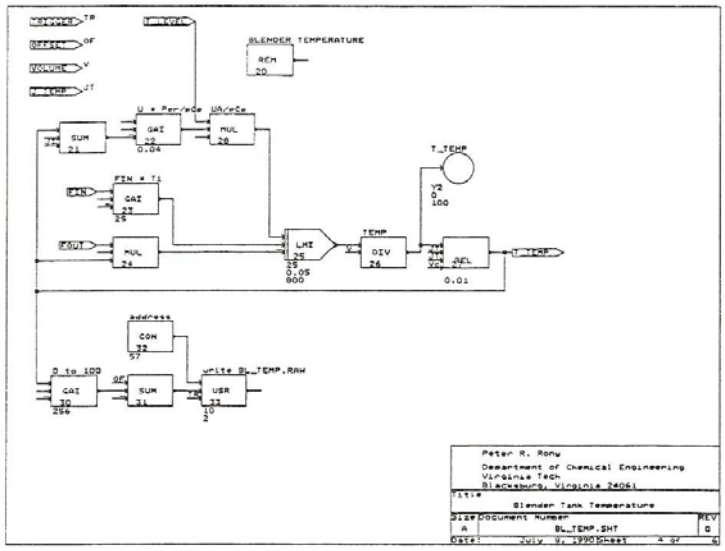


Figure 6

The TUTSIM/OrCARD diagram that represents that non-steady-state equation for the blender temperature

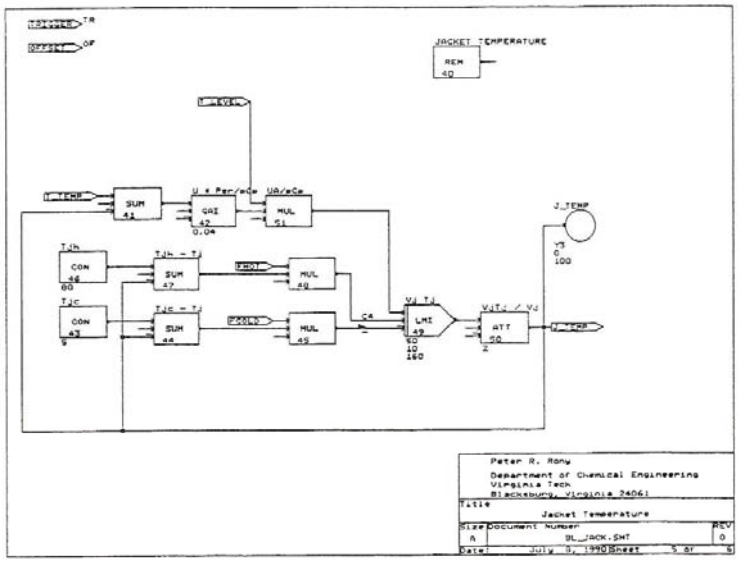


Figure 7

The TUTSIM/OrCAD diagram that represents the non-steady-state equation for the jacket temperature.

Results and Conclusions

In the control system development sequence described in [1], the blender process (Figure 2) was simulated in TUTSIM. In the TUTSIM simulation program, called BLENDER1.SIM, USR-block "hooks" were provided to the memory locations of the TI 500 Series PLC that executed the desired control strategy. The next step in the development sequence consisted of developing a regulatory control strategy in its simplest implementation: a single PID loop (for the tank temperature), a single analog alarm (for the tank level), and a few interlocks. The design of this simple regulatory control strategy was done at a high level, without the use of relay ladder logic (RLL), at best a difficult and inconvenient low-level language for chemical engineers.

Figure 9 depicts one result of our efforts: the closed-loop testing of the operation of the blender cold- and hot-water streams. The proportional gain was 2.6, the integral time was 1 min, and the four setpoints were 15 C, 35 C, 55 C, and 75 C. The multi-run capability of TUTSIM was used to make these plots. For additional details, the reader is directed to reference [1], a copy of which is available from the coauthor [4].

A somewhat similar, and perhaps competitive, approach to PID control simulation was described by Munkvold, McGlamery, and McLaughlin (University of Texas) in the Fall 1987 issue of CACHE News [5]. LabVIEW (Laboratory Virtual Instruments Engineering Workbench) software, which runs exclusively on the Macintosh, provides pulldown menus, multiple icons, and graphical case, iterative loop, sequence, and loop structures to provide a virtual instrument control panel and its underlying simulator diagram. These authors demonstrated how LabVIEW could be used to simulate the control of the liquid level in a tank by the manipulation of the input liquid flow rate in response to a level set point. For a recent discussion of LabVIEW's special features, please consult reference [6].

Clearly, TUTSIM/OrCAD, which execute on IBM-class personal computers, compare unfavorably with LabVIEW in the area of the user interface. Though OrCAD can use a mouse and does produce a TUTSIM block diagram that has some of the characteristics of the LabVIEW simulator diagram, TUTSIM only provides graphical (no grid) or tabular output for the user. LabVIEW icons such as switches, linear and rotary

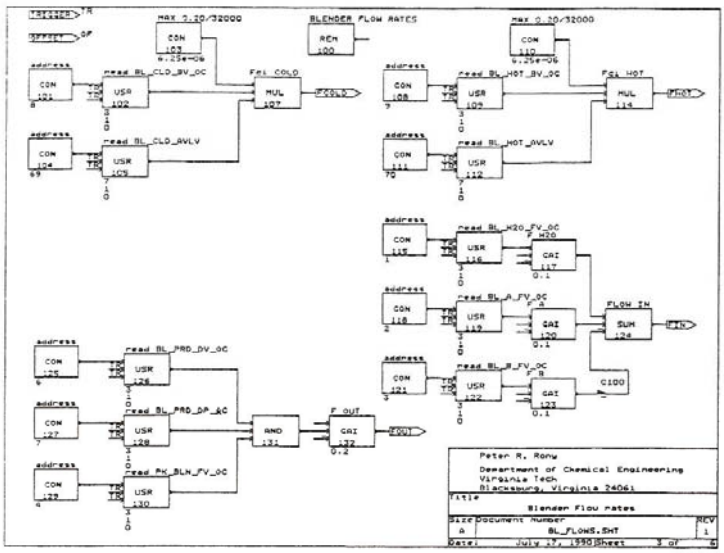


Figure 8

he TUTSIM/OrCAD diagram that represents the blender flow streams.

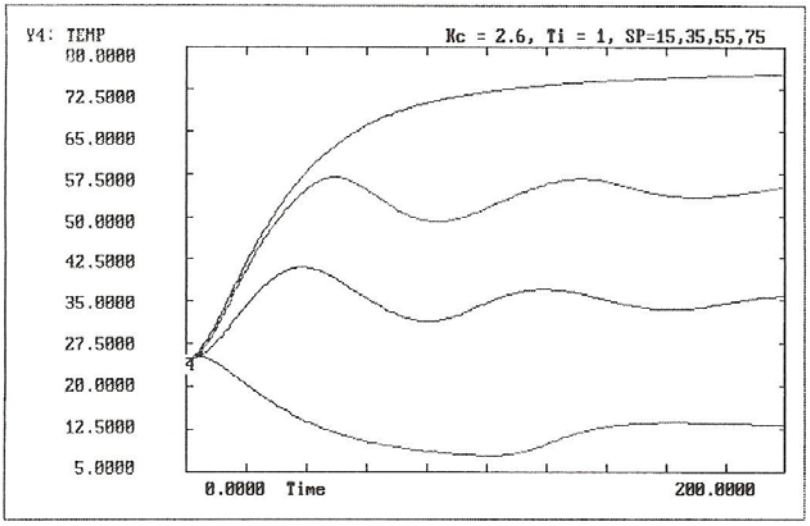


Figure 9

Closed-loop testing of the operation of the blender cold- and hot-water streams. The proportional gain was 2.6, the integral time was 1. min, and the four setpoints were 15 C, 35 C, 55 C, and 75 C.

potentiometers, bar graphs, null detectors, and digital indicators do not exist in TUTSIM. On the other hand, it is likely that the simulation of process models is easier to accomplish in TUTSIM, which has a simpler and perhaps more natural method of performing feedback than does LabVIEW. It may be that the analog-computer paradigm is more effective for the simulation of systems of ordinary and partial differential equations than the virtual-instrument paradigm. The author has had no experience with LabVIEW, so he can only speculate on this matter.

At the moment, TUTSIM possesses the advantage of being able to communicate with the memory locations of a Texas Instruments TI 500 Series of programmable logic controllers (PLC) [1]. A basic question associated with the design of PLC software is when to test the controller program logic, at startup or during the development of the code. For the latter alternative, TUTSIM is a software tool that permits the execution of the simulation and controller codes while they communicate with each other.

In combination, TUTSIM and the TI545 PLC (programmed using the APT high-level language) provide state-of-the-art capability in the implementation of inexpensive, midrange programmable logic controllers for the control of chemical processes. Best of all, such capability should be within the grasp of undergraduate chemical engineering students.

References

1. Contains excerpts from the article by Karl E. Rony and Peter R. Rony, "The TI 500 Series Programmable Logic Controllers: Merging of TUTSIM Dynamic Simulation With APT Control System Design," CAST Communications, 13 (2), Summer 1990.

2. For further details, contact TUTSIM Products, 200 California Avenue, #212, Palo Alto, CA 94306, (415) 325-4800.

3. Carlos A. Smith and Armando B. Corripio, "Principles and Practice of Automatic Process Control," Wiley, 1985, pp. 471-491.

4. Contact Karl Rony, APT Development Group, Texas Instruments Incorporated, Industrial Systems Division, Erwin Highway, P.O. Drawer 1255, Johnson City, TN 37605-1255, (800) 284-9084, extension 2078.

5. Glenn D. Munkvold, Gerald G. McGlamery, and Kevin J. McLaughlin (University of Texas), "PID Control Simulation Using LabVIEW," CACHE News (No. 25), 4-9, Fall 1987.

6. Michael Santori (National Instruments Corp.), "An instrument that isn't really," IEEE Spectrum 27 (8), 36-39 (August 1990).

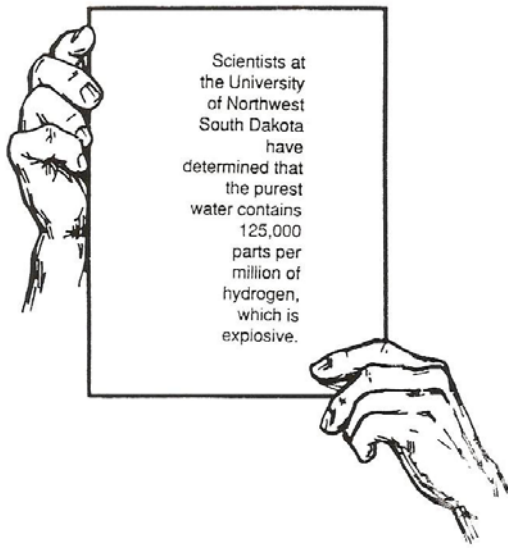


Table 1
TUTSIM listing of simulation program BLENDER1.SIM

```
PROFESSIONAL VERSION OF TUTSIM

Model File: BL1.SIM
Date:     7 /    21 /  1990
Time:    16 :    25
Timing:   1.0000     ,DELTA  ; 200.0000     ,RANGE
PlotBlocks and Scales:
Format:
      BlockNo,  Plot-MINimum,  Plot-MAXimum;  Comment
Horz:     0 ,    0.0000     , 200.0000     ; Time
  Y1:    26 ,   35.0000     ,  60.0000     ;  TEMP
  Y2:       ,               ,              ;
  Y3:       ,               ,              ;
  Y4:       ,               ,              ;


                    1 REM
;BLENDER PROCESS SIMULATION
   2.0000           2 CLK                          ; USR Trigger
   6.400E+03        3 CON                          ; OFFSET
                   10 REM
; VOLUME CALCULATION
   1.0000          11 LMI    124    -132           ; VOLUME
   0.0100000
  10.0000
   1.0000          12 CON                          ; Area
                   13 DIV     11      12           ; Level
   2.560E+03       14 GAI     13                   ; 0 to 10
                   15 SUM      3      14           ;
  58.0000          16 CON                          ; address
  10.0000          17 USR     16      15      2    ; write BL_LEVEL.RAW
   2.0000
   0.0000
                   20 REM
; BLENDER TEMPERATURE
                   21 SUM     27     -50           ;
   0.0400000       22 GAI    -21                   ; U * Per/pCp
  25.0000          23 GAI    124                   ; FIN * Ti
                   24 MUL    132      27           ;
  25.0000          25 LMI     28      23    -24    ;
   0.0500000
 800.0000
                   26 DIV     25      11           ; TEMP
   0.0100000       27 REL     26      50     50    ;
                              11
                   28 MUL     13      22           ; UA/pCp
 256.0000          30 GAI     27                   ; 0 to 100
                   31 SUM      3      30           ;
  57.0000          32 CON                          ; address
  10.0000          33 USR     32      31      2    ; write BL_TEMP.RAW
   2.0000
   0.0000
                   40 REM
; JACKET TEMPERATURE
                   41 SUM     27     -50           ;
   0.0400000       42 GAI     41                   ; U * Per/pCp
   5.0000          43 CON                          ; Tjc
                   44 SUM     43     -50           ; Tjc - Tj
                   45 MUL    107      44           ;
  80.0000          46 CON                          ; Tjh
                   47 SUM     46     -50           ; Tjh - Tj
                   48 MUL    114      47           ;
  50.0000          49 LMI     51      48     45    ; Vj Tj
  10.0000
 160.0000
   2.0000          50 ATT     49                   ; VjTj / Vj
                   51 MUL     13      42           ; UA/pCp
                  100 REM
  BLENDER FLOW RATES
   8.0000         101 CON                          ; address
   3.0000         102 USR    101       2      2    ; read BL_CLD_BV_OC
   1.0000
   0.0000
   6.250E-06      103 CON                          ; MAX 0.20/32000
  69.0000         104 CON                          ; address
   7.0000         105 USR    104       2      2    ; read BL_CLD_AVLV
   1.0000
   0.0000
                  107 MUL    103     102    105    ;Pci COLD
   9.0000         108 CON                          ; address
   3.0000         109 USR    108       2      2    ; read BL_HOT_BV_OC
   1.0000
   0.0000
   6.250E-06      110 CON                          ; MAX 0.20/32000
  70.0000         111 CON                          ; address
   7.0000         112 USR    111       2      2    ; read BL_HOT_AVLV
   1.0000
   0.0000
```

(continued on next page)

```
                114 MUL    110     109     112  ;Fci HOT
   1.0000       115 CON                         ; address
   3.0000       116 USR    115       2       2  ; read BL_H2O_FV_OC
   1.0000
   0.0000
   0.1000000    117 GAI    116                  ;F H2O
   2.0000       118 CON                         ; address
   3.0000       119 USR    118       2       2  ; read BL_A_FV_OC
   1.0000
   0.0000
   0.1000000    120 GAI    119                  ;F A
   3.0000       121 CON                         ; address
   3.0000       122 USR    121       2       2  ; read BL_B_FV_OC
   1.0000
   0.0000
   0.1000000    123 GAI    122                  ;F B
                124 SUM    117     120     123  ; FLOW IN
   6.0000       125 CON                         ; address
   3.0000       126 USR    125       2       2  ; read BL_PRD_DV_OC
   1.0000
   0.0000
   7.0000       127 CON                         ; address
   3.0000       128 USR    127       2       2  ; read BL_PRD_DP_OC
   1.0000
   0.0000
   4.0000       129 CON                         ; address
   3.0000       130 USR    129       2       2  ; read PK_BLN_FV_OC
   1.0000
   0.0000
                131 AND    126     128     130  ;
   0.2000000    132 GAI    131                  ; F OUT
                199 REM
; Controller Parameters
   1.0000       200 CON                         ; address
  50.0000       201 CON                         ; Setpoint
   1.0000       202 CON                         ; address
   5.0000       203 USR    200     201       2  ; write BL_TC.SP
   2.0000
   0.0000
   5.0000       204 USR    202       2       2  ; read BL_TC.SP
   1.0000
   0.0000
   5.0000       205 CON                         ; address
   3.1000       206 CON                         ; Prop Gain
   5.0000       207 CON                         ; address
   5.0000       208 USR    205     206       2  ; write BL_TC.KC
   2.0000
   0.0000
   5.0000       209 USR    207       2       2  ; read BL_TC.KC
   1.0000
   0.0000
   7.0000       210 CON                         ; address
   0.6000000    211 CON                         ; Int time
   7.0000       212 CON                         ; address
   5.0000       213 USR    210     211       2  ; write BL_TC.TI
   2.0000
   0.0000
   5.0000       214 USR    212       2       2  ; read BL_TC.TI
   1.0000
   0.0000
   9.0000       215 CON                         ; address
   0.1000000    216 CON                         ; Deriv Time
   9.0000       217 CON                         ; address
   5.0000       218 USR    215     216       2  ; write BL_TC.TD
   2.0000
   0.0000
   5.0000       219 USR    217       2       2  ; read BL_TC.TD
   1.0000
   0.0000
                999 SYC                         ;SYNC BLOCK
```

Distribution Committee Report

By Norman E. Rawson, IBM Corporation,
Brice Carnahan, University of Michigan,
Bruce A. Finlayson, University of Washington,
H. Scott Fogler, University of Michigan,
and Peter R. Rony, Virginia Tech.

An Ad Hoc Committee on Distribution was recently established to review distribution strategies for CACHE publications, software products and services. The objective was to determine if alternative distribution strategies could be more effective in reaching the users of CACHE products. Following is a summary of the committee's report.

PRODUCT DISTRIBUTION

Publications of Nominal Cost

It was determined that the cost for most publications is not a distribution consideration, and it was recommended that publications should be divided into the following classes prior to project approval:

- Class I - One free copy to each supporting institution
- Class II - Notification only to each supporting institution and one free copy upon request
- Class III - Licensed material and expensive material to be determined on a case-by-case basis

After initial distribution, a free copy will be provided to any individual from a supporting institution upon request. Nonsupporting institutions and student requests are charged a minimum of $25 or actual costs if greater. Each product should be reviewed for quality by the task force responsible for the product. The product quality review will use a checklist as its basis.

Software Distribution

It was suggested that CACHE produce a catalog of available software for use in chemical engineering classes categorized by subject matter. For the software to be included, it must be Generic software would only be included if it were used in a written by faculty or used by them in a course category. required course. Software written by students would be included; however, it must be reviewed and tested by a faculty member, and then submitted by the faculty member on behalf of the student.

Software chosen by CACHE will be distributed by notification to each institution with free distribution from a list server and/or diskette. The long term objective is to use only a list server. The contributing party would be responsible to test the program and documentation by down loading it from the list server. Another site(s) would also be required to down load and test the program prior to announcement. Documentation will be down loaded from the list server wherever practical.

Software requiring a license fee or costly software would be determined on a case-by-case basis. It could be either distributed from the licensing institution, fee collected by CACHE and forwarded to the licensor, or distributed from CACHE once the fee has been received. CACHE should be the one point of control for software delivery and maintain accounting records, licensing fees, etc. A trial period for a fee refund would be established, if required. In some, cases a continuing fee would also be used when necessary to satisfy licenses or continued development and maintenance.

Education Product Testing

A future means of product evaluation could be the electronic solicitation of student response to CACHE programs. CAI modules should automatically offer students an opportunity for comment, and the student comments should be summarized locally and E-mailed to the responsible task force which delivered the product. A form of electronic feedback should be established in 1991. Development of a general data gathering facility for incorporation into any program is also feasible. Gathering and summarizing the results of such surveys for feedback is more complicated and requires a facility management program. Before such a system development is undertaken, CACHE should be sure mechanisms are in place to make effective use of the feedback.

Electronic Distribution

The committee's vision was one of electronic distribution. Electronic distribution has the potential to give CACHE products increased publicity and ease of access. Greatly increased network speeds and the rapid movement toward open systems will make electronic distribution very practical by the mid-90's. Some forms of electronic distribution are feasible today. Its use should be encouraged wherever network speeds are not an inhibitor, general interchangeability can be established and sufficient product demand exists to warrant use electronic distribution.

Source Program transmission can usually be satisfied by using ASCII format and network transmission is straightforward. Object Program files are transmitted in binary format and network transmission is generally straightforward, however, conversion and packing/unpacking functions are required to bypass character restrictions in some network protocols. The Open Software Foundation has issued a RFT (Request for Technology) to select an Architecturally Neutral Distribution Format (ANDF) solution by mid-1991. This should solve many architectural incompatibility problems.

While electronic documentation is entirely feasible today, several potential problem areas exist. Larger documents containing graphics or binary files will require higher data transmission speeds than most networks use today. T1 speed (1.5 megabits per second) is preferred. Since NSFNET is moving to T3 speed (45 megabits per second), the backbone network will be in place shortly. Some local campus networks and workstation storage may have to be upgraded to handle large documents effectively. Tests of networking capabilities should be undertaken in 1991.

A second and potentially greater problem with electronic documentation is the lack of standardization. Each word processor and text processor uses its own coding scheme, making interchangeability dependent on proper conversion. The coding schemes fall into two categories, procedural or descriptive markup. Procedural markup codes the keystroke transactions of a word processor (eg: indent, tab, end of line, etc.). It is dependent on the WYSIWYG procedure of the interactive input and cannot be standardized, since it is personalized to the inputting process for the specific word processor. Descriptive markup can form a basis for a standard since it is not related to the inputting process, but separates the format of the document from the content and can conform to a standard syntax.

Descriptive markup can be used to define the logical structure of the document apart from the information instance, and uses descriptive markup tags to define the document elements in a generic sense. It can be used to interchange documents and separate the document content and structure from the hardware and software being used to print, display or revise the document. One form of descriptive markup is Standard Generalized Markup Language (SGML). SGML will probably provide the future basis for document interchange and electronic publishing; however, it is not evident that SGML based WYSIWYG editors capable of mathematical formula processing, graphics and image will be available in the near term. Today's WYSIWYG editor products generally provide limited import of ASCII text. Mathematics, graphics and image capability are not uniformly available or implemented in a standard fashion. Bidirectional import and export to foreign word processors or publishing products is usually not available, making revisions difficult. This situation is expected to improve as standards develop.

In the interim period, two possibilities for document distribution are:

1. Use of Postscript as a basis. This would not allow for revision capability, but would allow all computers with Postscript capability to down load and print the document, provided a reasonable standard was followed to avoid local personalization. Documents with a low image content should work well, however, documents with many images can become quite large and potentially could create some performance problems.

2. Use a standard set of documentation, storage and editing programs run on a CACHE "client" system (WS or host), with resultant output "served" up with X-windows to the user WS's and PC's. This wouldallow both document interchange and revision capability. It would be far more restrictive, however, since the user's workstation would require support of X-Windows and would have to use the standard document program set chosen by CACHE. In addition, a high speed network would be required for effective interactive computing.

The committee suggests that a staged approach and feasibility testing should be initiated in 1991 to understand the practical limitations of today's technology, and to be prepared to make future use of standards as they progress.

PUBLICITY

Use of AIChE

The committee recommended greater use of AIChE to announce and advertise high volume CACHE products in CEP. A section on CACHE products should be included in the ANNUAL SOFTWARE DIRECTORY OF CHEMICAL

ENGINEERING PROGRESS. The CHAPTER ONE AICHE publication should also be used to reach local sections and students. Regular CACHE Tutorials should be scheduled at AIChE meetings, and CACHE should have a table displaying CACHE products at the annual AIChE meeting. CACHE should investigate the use of AIChE distribution for large volume items.

Use of Internet for Publicity

Greater use of Internet should be investigated for distribution of CACHE products. It was suggested that new products should be announced via BITNET/Internet. A central distribution file server for more detailed information should be referenced in all publicity, and supported for each CACHE product at time of announcement. Computer Conferencing has the potential to increase communication and productivity with users of CACHE products and should be tested on a new product in the future.

ELECTRONIC COMMUNICATIONS

CACHE Must Promote the Vision of a Networked ChE Community

Communications capability will dramatically increase in the 90's and the Internet will provide broad access to industry and universities. Open systems standards will allow interoperability and electronic mail will be established throughout the chemical engineering community. The Electronic Mail Task Force should add sources with expertise to consult and provide guidance in electronic communications. CACHE should conduct tests for interoperability and establish guidelines for mail and document distribution. In addition, a wide area electronic server should be established. LSU plans to test a list server for simple requests of files. CACHE should test this facility and evaluate its use.

CACHE should lead in conducting business electronically. It should use E-mail for routine correspondence among trustees and maintain a central directory for user ID's for Chemical Engineering Departments, faculty, AIChE staff, CAST Division staff and AIChE Student Chapters/key students. All Chemical Engineering Departments should be encouraged to participate and establish "at desk" BITNET support to every faculty member. CACHE should include an E-mail address on stationery and publications. E-mail addresses should be in the CHEMICAL ENGINEERING FACULTY HANDBOOK.

It is particularly important that AIChE be encouraged to use E-mail. CACHE should use E-mail with AIChE headquarters and Council on projects of mutual interest, and encourage AIChE to use E-mail for their routine communications to committees, etc. CACHE should assist in establishing a wide area server for AIChE (either AIChE's, LSU, or future CACHE system). The Electronic Mail Task Force plans to conduct tests of E-mail formats to enable common distribution of minutes and business correspondence to CACHE Trustees.

CONFERENCES

Electronic Conference Facilitation

An electronic conference data base will be practical, when most of our domestic and international conference attendees are regular E-mail users with access to electronic message services over the Internet. Conference applications could then be submitted via E-mail. Information for creating a conference data base (name, address, phone, E-mail address, etc.) could be retrieved from E-mail submission using cut and paste operations, and confirmation could be sent immediately. Notices of most conference arrangements could be handled electronically, however, fees would still be sent by mail and receipted electronically.

Electronic Distribution of Conference Programs and Documents

Electronic assistance to conference arrangements can improve productivity. Abstract submission could be standard ASCII format, submitted via E-mail and handled electronically. Word processor and graphics file formats should be investigated and a standard base support set should be determined to collect manuscripts electronically. Several style sheets will be investigated for inputting conference papers from common word processors and publishing programs.

By the mid-90's, SGML might serve as the base for paper submission, proceedings publication and as the document retention standard. Document requests could be filled and proceedings published electronically. Tests should be conducted so that electronic facilitation of conferences can proceed as the capability develops. Other standards work should be followed. For example, a Professional Publishing Interchange Standards Committee is defining a Page Interchange Language (PIL) to facilitate electronic interchange of published products. Some organizations are also defining standard SGML Document Type Definitions (DTD's) for document submission. CACHE should test the more promising standards in view of their potential use for FOCAPD in 1994.

An Overview of Commercially Available Software for Distillation Extraction, Adsorption, and Membrane Processes

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SUMMARY

In recent years there has been an explosion of commercially available software for both mainframe and personal computers. Software for solution to separations related problems are part of this trend. Many programs are available for distillation; less for extraction and adsorption processes; and a limited number for membrane processes.

Objectives of this paper are to present an overview of: (1) software available, (2) specific separation problems which can be solved, (3) characteristics for selected programs, (4) hardware requirements, and (5) software suppliers.

INTRODUCTION

Highlights of commercially available software for separations are presented in Table I. Further details on each program follow. In some cases costs are given but we recommend suppliers be contacted directly for cost information, details on the capability of specific programs, and the extent of technical support provided.

ADSIM/SU is a rigorous simulator for adsorption processes offered by ProsysTech, Inc. (Florham Park, New Jersey). Adsim uses a variety of pressure driven algorithms to model these processes. The program has a library of all the commonly encountered unit operations, each incorporating heat and material balances. ADSIM/SU can perform a simulation or design of a pressure and temperature swing adsorption unit. This program also links to SPEEDUP for process flowsheeting. ADSIM/SU has a cycle manager that controls the opening and closing of valves that is carried out in pressure swing adsorption (PSA) plants. Output produced is in table and plot form. The program also allows for user added models. ADSIM/SU is available for use on both the Digital VAX and IBM computers.

ADSORB

ADSORB is an adsorption simulator developed by Kenneth A. Wilde (Austin, Texas). This program simulates adsorbent and ion exchange beds. It requires an IBM PC or compatible with DOS 2.1 or later, 320K RAM, one disk drive or hard drive, and may be used with any type printer. AT hardware and/or an accelerator board will shorten run times significantly. Data may be entered from input/edit menus with error trapping or from previously saved disk files. Data requirements include stream flows, bed size, particle size and density, pure component fluid solid isotherms, and transport data. Computations for a regeneration/exhaustion cycle with four components will take 5-20 minutes.

The program solves the partial differential equations governing each of the components. The full Ideal Adsorbed Solution Model is used for activated carbon. The effect of multicomponent interaction and concentration dependence are included. In December 1989, the cost was $895 for one application, $1095 for two and $1195 for three. The three areas covered are aqueous adsorption, gas adsorption and ion exchange.

AMSIM

AMSIM is a steady-state absorption simulator developed by DB Robinson & Associates Ltd. (Edmonton, Alberta Canada). It utilizes a rigorous non-equilibrium stage model to simulate alkanolamine-based systems used to remove carbon dioxide and hydrogen sulfide from gaseous hydrocarbon streams. The non-equilibrium stage model applies a stage efficiency to individual components. Using a modified Murphree vapor stage efficiency, the model independently characterizes the composition of each component on any stage within the absorber or regenerator.

TABLE I
SUMMARY OF COMMERCIALLY AVAILABLE SOFTWARE

DISTILLATION / ABSORPTION / STRIPPING			
SOFTWARE	*SUPPLIER ADDRESS*	*TELEPHONE/FAX*	*COMMENTS*
AMSIM Column	DB Robinson & Associates Ltd. 9419 - 20 Avenue Edmonton, Alberta Canada T6N 1E5	(403) 463-8638 Telex - 037 2966	AMSIM is specialized for non-equilibrium simulation of alkanolamine processes. Column simulates fractionators using the Ishii-Otto algorithm.
ASPEN PLUS* BATCHFRAC	Aspen Technology, Inc. 251 Vassar Street Cambridge, Massachusetts 02139	(617) 497-9010 Fax - (617) 497-7806 Telex - 948 038	ASPEN PLUS is a flowsheet simulator without dimensional limitations. Also available: RATEFRAC & BATCHFRAC for rate-based and batch distillations.
ASPEN/SP*	JSD Simulation Service Company** 6000 East Evans Avenue Bldg. 3 Denver, Colorado 80222	(303) 758-6862 Fax - (303) 692-0757	ASPEN/SP is a flowsheet simulator that uses an inside out algorithm for rigorous distillation. No limits on flowsheet size.
BASIS	Engineering MicroSimulations Inc. P.O. Box 543 Storrs, Connecticut 06268	(213) 429-4218	BASIS is a rigorous batch distillation simulator that allows tracking of the distillation in progress. Database contains 80 common chemicals.
BR & E programs	Bryan Research & Engineering, Inc. P.O. Box 3403 Bryan, Texas 77805	(409) 846-8771 Fax - (409) 846-8811	TSWEET is an amine plant simulation program. PROSIM is a general simulator for common processes. DEHY is a simulator for glycol dehydration plants.
CHEMCAD II*	COADE/CHEMSTATIONS, Inc. 10375 Richmond Ave. Suite 1225 Houston, Texas 77042	(713) 954-4100 Fax - (713) 954-4099 Telex - 415 866	CHEMCAD II is a flowsheet simulator for use on a PC. The data bank has over 650 compounds and experimental data may be used with programs regression package.
CHEMCALC 1 CHEMCALC 11 CHEMCALC 16	Gulf Publishing Company 3301 Allen Parkway Houston, Texas 77019	(713) 520-4444 Fax - (713) 520-4438 Telex - 275 418	CHEMCALC 1 calculates min. trays, reflux, flashes,etc. CHEMCALC 11 is an amine process simulator. CHEMCALC 16 is a liquid-liquid extraction simulator.
DESIGN II*	ChemShare Corporation P.O. Box 1885 Houston, Texas 77251	(713) 627-8945 Fax - (713) 965-0968	DESIGN II is a flowsheet simulator with graphical output, a data bank of 870 compounds, and a crude library of 150 published crudes. Phase envelope ability.
DIST	Paul Barton, P.E. Box 158 Road 4 Bellefonte, Pennsylvania 16823	(814) 355-0312	DIST is an interactive, semi-rigorous distillation package for multi-component distillation. Program performs a stage-to-stage bottom to top procedure.
DISTIL SIMU	Engrsoft 1946 Holland Wichita, Kansas 67212	(316) 721-1598	DISTIL SIMU generates a McCabe-Thiele diagram and steps off stages. Also included is a nonlinear regression package for regressing sets of X,Y data.
Source: J. L. Humphrey & Associates (Austin, Texas)			

TABLE I
SUMMARY OF COMMERCIALLY AVAILABLE SOFTWARE

DISTILLATION / ABSORPTION / STRIPPING, Continued			
SOFTWARE	*SUPPLIER ADDRESS*	*TELEPHONE/FAX*	*COMMENTS*
ELECTRONIC DESIGN MANUAL	Nutter Engineering Div. 639-T W. 41 st Tulsa, OK 74170	(800) 331-4462 Fax (918) 446-5321	ELECTRONIC DESIGN MANUAL predicts hydraulic performance of Nutter's trays and packings.
HYSIM*	Hyprotech 2500 Citywest Blvd. Suite #300 Houston, Texas 77042	(713) 780-7087 Fax (780) 780-9504	HYSIM is a flowsheet simulator that uses interactive menus. Database contains over 800 compounds. Programmed in C. No limit on flowsheet size.
Norton Packed Tower Design Program	Norton Company P.O. Box 350 Akron, Ohio 44309	(216) 673-5860	NORTON PACKED TOWER DESIGN PROGRAM estimates the required column diameter and height for columns utilizing Norton's packings.
PD-PLUS	Deerhaven Technical Software 7 Shady Lane Drive Burlington, Massachusetts 01803	(617) 229-2541	PD-PLUS is a PC-based flowsheet simulator. It has a component library with 59 compounds & handles up to 60 components, 300 streams, & 100 equilibrium stages.
PROCESS/ PROPII*	Simulation Sciences, Inc. 1051 West Bastanchury Road Fullerton, California 92633	(714) 879-9180	PROCESS/PROII are flowsheet simulators that use key-word file & fill-in menus for data input. Several models available for distillation.
SPARO	Kesler Engineering, Inc. 320 Raritan Avenue Highland Park, New Jersey 08904	(201) 545-6000 Telex - 844 544	SPARO is a flowsheet process analysis system that can be customized to individual needs. Handles up to 50 unit operations, 100 streams, & 50 components.
SPEEDUP	ProsysTech, Inc. 30 Vreeland Road Florham Park, New Jersey 07932	(201) 377-4855 Fax - (201) 377-7355 Telex - 132 265	SPEEDUP is an integrated process simulator that uses an equation-oriented structure for both steady and unsteady state processes. Generates reports and graphic output.
SULPAK-PC	Sulzer Brothers Limited CH-8401 Winterthur, Switzerland (052) 81 11 22	(052) 81 11 22 Fax - (052) 23 56 97 Telex - 896 060 66	SULPAK-PC is a distillation sizing and design program for columns filled with Sulzer packings.
TECS programs	TECS software, inc P.O. Box 720730 Houston, Texas 77272	(713) 561-6143 Telex - 6503090217	DISTIL-S, DISTIL2, DISTIL-R are programs for shorcut & rigorous distillation simulation. PACKTWR calculates the diameter and pressure drop of packed towers. SWS1 determines the number of trays required for ammonia and hydrogen sulfide reduction in sour water stripping. VALTRAYG designs and rates valve trays of up to 5 passes. AMINE1 for amine plant modeling. MOLSIEVE for gas dehydrator plants.
Source: J. L. Humphrey & Associates (Austin, Texas)			

*These programs are the largest of the system simulators. They generally contain a thermodynamic data bank and other supporting functions.

**Acquired by Simulation Sciences, Inc.

TABLE I
SUMMARY OF COMMERCIALLY AVAILABLE SOFTWARE

EXTRACTION			
SOFTWARE	*SUPPLIER ADDRESS*	*TELEPHONE/FAX*	*COMMENTS*
ASPEN PLUS	Aspen Technology, Inc.	(617) 497-9010	Rigorous multistage liquid-liquid extraction.
ASPEN/SP	JSD Simulation Service Company	(303) 758-6862	Rigorous multistage liquid-liquid extraction.
CHEMCAD II	COADE/CHEMSTATIONS, Inc.	(713) 954-4100	Rigorous multistage liquid-liquid extraction using an enhanced verison of the sumultaneous correction algorithm.
PROCESS/ PROII	Simulation Sciences, Inc.	(714) 879-9180	Rigorous multistage liquid-liquid extraction with the modified Sujata or Naphtale-Sandholm technique.
Source: J. L. Humphrey & Associates (Austin, Texas)			

ADSORPTION			
SOFTWARE	*SUPPLIER ADDRESS*	*TELEPHONE/FAX*	*COMMENTS*
ADSIM/SU	ProsysTech, Inc.	(201) 377-4855	Rigorous modeling of adsorption beds with SPEEDUP interface using pressure driven algorithms.
ADSORB	Kenneth A. Wilde 3604 Laurel Ledge Lane Austin, Texas 78731	(512) 452-6613	ADSORB simulates adsorption/regeneration for the areas of aqueous adsorption, gas adsorption and ion exchange.
ProChem	OLI Systems, Inc. 135 Columbia Turnpike Suite #201 Florham Park, New Jersey 07932	(201) 514-1290	Specialized simulator for interphase equilibria that may be used to model ion exchange chromotography and other adsorption processes.
Source: J. L. Humphrey & Associates (Austin, Texas)			

MEMBRANES			
SOFTWARE	*SUPPLIER ADDRESS*	*TELEPHONE/FAX*	*COMMENTS*
ASPEN PLUS	Aspen Technology, Inc.	(617) 497-9010	Models solid-liquid separations like ultrafiltration.
PROCESS/ PROII	Simulation Sciences, Inc.	(714) 879-9180	Permeation membranes models: classical spiral wound and hollow-fiber mermbranes.
Source: J. L. Humphrey & Associates (Austin, Texas)			

Combining the stage efficiency with the material and energy balances for each column, a system of non-linear algebraic equations is generated and solved. A component library containing 14 commonly encountered chemicals in the natural gas processing industry is available. The solubility and kinetic parameters used by the program are based on experimental data. Minimum hardware requirements are a PC or compatible with 512K RAM, MS-DOS 2.0, math coprocessor, and two 360 KB floppy drives or one floppy and one 10 MB hard drive.

ASPEN PLUS

ASPEN PLUS is a flowsheet simulator created by Aspen Technology, Inc. (Cambridge, Massachusetts). Input is entered using a keyword format. The output from the model includes a stream summary and a report for each unit operation block, and optionally, the cost and economics of the process. The user may also add in-line FORTRAN statements and subroutines into the flowsheet computations. There are no dimensional limitations on simulations.

It is capable of modeling vapor-liquid phase equilibrium, absorption, stripping, liquid-liquid extraction, extractive, azeotropic, and ordinary distillation. The program is also capable of modeling some solids separations and liquid-solid separations. The user can also order Aspen Tech's new rate-based separations model, RATEFRAC. This recently developed model is a rate-based nonequilibrium model that simulates separation columns based on actual trays and real packings rather than the combination of equilibrium stages and stage efficiency. Aspen Tech also markets BATCHFRAC, a rigorous unsteady-state model for batch distillation. Like RATEFRAC, this model can be added to the ASPEN PLUS package.

The physical property models library is extensive. A pure component library contains nearly 500 components. Property models are available based on both the equation of state and activity coefficient approaches. The program also allows user supplied data banks for proprietary parameters. It also has a property generator that produces detailed plots and tables of physical property results, including a P-T phase envelope diagram. The program can be installed on PC and SUN computer systems.

ASPEN/SP

ASPEN/SP is a steady state flowsheet simulator developed by JSD Simulation Service Co. (Denver, Colorado). Input is entered using a keyword file. Output includes graphics capabilities. The separations processes that can be modelled include distillation, absorption, stripping, shortcut distillation, and solids processes such as Venturi scrubbers, cyclones, and others. The primary distillation model is RADFRC, a rigorous stagewise program. This model can handle any number of stages and components. RADFRC is based on an inside-out algorithm. The flash capabilities of ASPEN/SP include one, two, and three phase flash units, including those with electrolytes and solids.

ASPEN/SP has an extensive physical properties library including a binary data library compiled by DECHEMA. ASPEN/SP allows the user to add FORTRAN statements, including subroutines, to the program. ASPEN/SP is available for both mainframe and PC systems. Workstation versions are available for VaxStations, Apollos, and Sun systems. ASPEN/SP is available for 386-based PC's.

BASIS

BASIS is a rigorous batch distillation simulation designed for use on a PC marketed by Engineering Microsimulations Inc. (Stom, Connecticut). Input is entered via pop-up menus. A continually updated display enables user to track the distillation in progress, adding material or dumping the accumulator, changing the pressure profile, boil-up rate, or distillate rate at any time. The thermodynamic database contains 80 common chemicals and rigorous correlation for representing highly non-ideal mixtures. The virial equation of state is used to calculate vapor phase properties while the NRTL equation is used for liquid phase activity coefficients. The program allows the user to add to the thermodynamics data base available for the PC with 320 K memory and a math coprocessor.

BRYAN RESEARCH & ENGINEERING

The following programs are marketed by Bryan Research & Engineering (Bryan, Texas). They are available for both mainframe and personal computers.

TSWEET - A process simulation program for amine gas and/or liquid sweetening plants. The program can handle applications for several types of amine solvents. It solves problems by rigorous stage-to-stage calculations for the contactor and regenerator columns. The program allows multiple absorbers in series or parallel, interstage heating/cooling, multiple feeds and withdrawals. The interactive graphics enable the user to draw a flowsheet on the screen which is used to enter operating data on pop-up forms.

PROSIM - A general purpose simulator that performs complete mass and energy balances for common processes. Available separation unit operations include absorbers, strippers, and distillation columns. The program uses the same interactive graphics for data input as Tsweet.

DEHY - A process simulator for glycol dehydration plants. The program performs rigorous stage-to-stage calculations in the contactor and regenerator. Program handles several types of glycols. It allows a secondary glycol stripper to produce leaner glycol. It has the same interactive graphics as TSWEET.

CHEMCAD II

CHEMCAD II is a flowsheet simulator offered by Coade/Chemstations, Inc. (Houston, Texas) for use on PC's with math coprocessors, MS-DOS 3.0 or higher is required. CHEMCAD II offers both graphical and interactive user interfaces. It also has an interactive simulator, TALK, which provides fill-in-the-blank menus. The user can perform calculations for the entire system, or just for individual processes within the system. Output can be in the form of process flow diagrams, or in report form.

CHEMCAD II has a extensive set of thermodynamic options for calculating liquid/liquid and liquid/vapor and vapor/liquid/liquid equilibrium including UNIFAC parameters. The component data bank stores 650 components and calculates equilibria for non-ideal systems without the need for experimental data. Experimental data may be used with the built-in regression package.

Separations operations include batch, rigorous and shortcut distillation, liquid-liquid extraction, and two and three phase flash vaporization. The rigorous distillation can use an enhanced inside-out algorithm or a Newton-Raphson simultaneous correction method. The liquid/liquid extraction model uses an enhanced version of the simultaneous correction algorithm to rigorously perform the heat and material balance of immiscible liquid mixtures. The size constraints on these columns are 5 feeds, 6 products, and 300 stages. The user may also add their own unit operations, K-value options, and enthalpy options.

CHEMCALC PROGRAMS

The following programs are available from the Gulf Publishing Company (Houston, Texas).

• CHEMCALC 1 Separations Calculations - Determines conditions and compositions of multi-component mixtures at the dew point and bubble point. Performs binary and multi-component flash calculations. Also calculates minimum trays and reflux for multi-component separations based on the light and heavy keys. Actual trays are calculated based on the Erbar-Maddox correlation. This program requires 256K RAM and 2 disk drives.

• CHEMCALC 11 Amine Process Simulator - Models processes for absorption or stripping of hydrogen sulfide and carbon dioxide from gas streams. For hydrocarbon gases, the program determines the amount of hydrocarbons stripped and absorbed. This program determines the required amine circulation rate, pressure and temperature conditions, and number of theoretical stages. Several of the common amines may be used. For reaction purposes, the Kent-Ersenberg model is used. This program requires 256K RAM and 1 disk drive.

• CHEMCALC 16 Liquid-Liquid Extraction - Determines material balance, number of theoretical stages, and stage efficiency in extraction operations. Examples of applications include solvent dewaxing, propane decarbonizing, gas sweetening and crude oil dewaxing. Requires 240K RAM and 1 disk drive.

DESIGN II

DESIGN II is an integrated flowsheet simulator offered by the ChemShare Corporation (Houston, Texas). Versions of this program are available for both mainframe and personal computers. The program has an input processor program allowing the user to create files from detailed menus and fill-in screens. The user can stop calculations in progress and review interim results. Output can be presented in graphical form.

The program has an extensive data bank with 870 pure components, 27 K-value options, and 22 enthalpy options. The crude library has over 150 published crudes. There are no limits on flowsheet size, columns size, trays, components, feeds, and products. The user may add in-line Fortran statements and thermodynamic correlations

Separations available are rigorous and shortcut distillation, absorption, stripping, and flash operations. The program has two convergence methods available. Phase envelopes may be generated using the SOAVE equation of state.

DIST

DIST is the software package for the BASIC computer program marketed by Paul Barton, P.E. (Bellefonte, Pennsylvania). DIST is an interactive semi-rigorous, multi-component distillation package that can be used to model continuous, steady state, fractional distillation problems. The program calculates the stage requirements needed to accomplish a separation. The program runs on PC's with a minimum of 256K RAM.

The method used is a stage-to-stage calculation, that solves material, heat and equilibrium equations. Output contains number of theoretical stages, temperature, pressure, vapor and liquid flow rates for each stage, feed stage location, feed and product rates and compositions. The program can handle up to 10 components and 100 equilibrium stages.

DISTIL SIMU

DISTILL SIMU is an interactive McCabe-Thiele simulator offered by ENGRSOFT (Wichita, Kansas). Input data can be entered using menus and is completely interactive. Output data includes input specifications, minimum reflux ratio, number of equilibrium stages and a McCabe Thiele graphic diagram. The program is written using Microsoft's QuickBasic 4.0 and is designed to run on a PC with 512K RAM, hard disk, DOS 3.0 or later.

DISTIL SIMU may be used to predict the relative volatility, perform a nonrigorous distillation simulation or provide vapor-liquid equilibria (VLE) curve fitting. The distillation program is limited to binary systems requiring less than one hundred equilibrium stages. Because of the graphics output, this program is very useful for teaching purposes.

ELECTRONIC DESIGN MANUAL

ELECTRONIC DESIGN MANUAL is a design program developed by Nutter Engineering (Tulsa, Oklahoma). This program predicts the distillation performance of Nutter's trays and packings. The program requires any IBM PC or compatible computer.

HYSIM

HYSIM is a comprehensive flowsheet simulator offered by Hyprotech Ltd. (Houston, Texas). Data can be entered using menus and is completely interactive. Output includes stream summaries, column results and specifications. Graphical output includes process flow diagrams, phase envelopes, and pinch analyses. It can be run on a mainframe or PC with 512K RAM, a math coprocessor, hard disk, and DOS 3.0 or higher.

The separations processes available include rigorous distillation, shortcut distillation, and flash vaporization. The database has over 800 components. The user can also add to the library. Extensive thermodynamics capabilities are available including SRK, and Peng-Robinson equations of state. Liquid activity methods which are available include the Margules, UNIQUAC, NRTL, Van Laar, and Wilson, as well as many other thermodynarnic correlations.

NORTON PACKED TOWER DESIGN PROGRAM

NORTON PACKED TOWER DESIGN PROGRAM was developed by the Norton Company (Akron, Ohio). The program estimates column diameter and packing efficiency for Intalox(~) metal tower packing and Intalox structured packing. The program is designed to run on a PC with 512K RAM hard disk, DOS 3.0 or later..

This program calculates the performance of a distillation tower filled with either Intalox metal tower packing or Intalox structured tower packing at different column loadings. The efficiency (HETS) of the Intalox metal tower packing is predicted from an empirical correlation developed which is a function of the packing size, surface tension and the liquid viscosity. The program includes typical organic HETS's for the Intalox 2T structured packing. The correlation is limited to systems with a relative volatility of 3 or less. Pressure drop is calculated using the 1985 updated version of the Eckert modification of the Sherwood, Shipley and Holloway correlation. The column diameter is calculated based on 80% of the maximum capacity.

PD+PLUS

PD-PLUS is a PC-based program for simulating chemical processes and was developed by Deerhaven Technical Software (Burlington, Massachusetts). Separations processes available include fractionators, absorbers, strippers, crude and vacuum columns, and a flash vaporization. Hardware requirements are a PC with 640K RAM, math coprocessor, and an operating system of DOS 2.0 or higher.

Input is entered in a keyword-based format. The interactive ability of the program allows the user to stop the program as the next calculation step is about to begin and display stream properties. The component library includes 59 compounds, but an optional 1,023 component version is available. Thermodynamic K-values are calculated by the program using general correlations, by ideal K-values plus liquid activity coefficients, or by user-supplied data. Limitations are 60 components, 300 streams, and 100 equilibrium stages.

PROCESS/PRO II

PROCESS/PROII are flowsheet simulators that use keyword and menu-driven inputs, respectively. This software is offered by Simulation Sciences Inc. (Fullerton, California). In addition to ancillary operations, Process/ProII offers the following separation models: rigorous and shortcut distillation, liquid-liquid extraction, and permeation membranes. The rigorous distillation models available use the following solution techniques: Newton Raphson, Modified Thiele-Gedes, Inside-Out, Wang Henke, and modified Naphtale-Sandholm. The available models for liquid-liquid extraction are the modified Sujata technique, and a modified Naphtale-Sandholm technique. Shortcut models include Fenske, Underwood, and Gilliland-Kirkbride. The permeation membrane models are applicable to classical spiral wound and hollow-fibers.

These programs offer extensive physical property models and a large component library. PROCESSIPROII is available for mainframes and personal computers.

SPARO

SPARO is a flowsheet process analysis system for refinery, petrochemical, and gas processing operations offered by Kesler Engineering, Inc. (Highland Park, New Jersey). The program can be customized to meet the individual user's needs. This PC-based simulator gathers input by using self-prompting menus.

The main program is SPAN, which performs separations simulations for distillation, flash vaporizations, and provides phase envelopes. MAXSTILL is the model within SPAN that performs stage-to-stage calculations for distillation columns. KFLASH is used to predict vapor-liquid equilibria. SPAN has "pinchpoint" analysis capability. Limits on flowsheet size are 50 unit operations, 100 streams, and 50 components. The program will run on PC's with 640K of RAM, a hard disk, and a math coprocessor.

SPEEDUP

SPEEDUP is an integrated process simulator developed by ProsysTech, Inc. (Florham Park, New Jersey). Input is entered interactively. The user can add models to the program.

Available separations include rigorous and shortcut distillation, and flash operations. The program allows the user to link physical properties to the thermodynamics calculation procedures of the user's choice. SPEEDUP is written in PASCAL and FORTRAN 77. It is available for PC and VAX computers.

SULPAK-PC

SULPAK-PC was developed by the Sulzer Brothers, Limited (Winterthur, Switzerland). Sulpak-PC is a design and sizing program for distillation and absorption columns which utilize Sulzer packings. This program runs on any PC using DOS 2.0 or higher, with one disk or hard drive, and 150K of RAM.

In the DESIGN mode, the shortcut method is used to estimate the minimum reflux ratio, vapor and liquid loads and number of theoretical stages for up to 5 components.

In the SIZING mode, absorption and distillation are treated separately. Values of distillation efficiencies of different packings are given for organic systems. Capacity data are provided for distillation and absorption. The capacity prediction for distillation is based on organic systems, while absorption and stripping capacity estimation is based on the air/water system. The following restrictions apply for this program:

- pressure < 2 bar
- relative volatilities < 3
- well-wetting organic systems
- viscosity < 5 cP
- surface tension > 5 dynes/cm

TECS PROGRAMS

Technical Computing and Simulation (Houston, Texas) separations programs are designed to run on PC's. These programs include the following simulators:

Distil-S - Shortcut distillation program that calculates the minimum reflux ratio, minimum number of theoretical sages, reflux ratio, number of theoretical stages, and optimum feed tray location using user supplied input of feed condition, composition, and relative volatilities.

Distil2 - Similar to Distil-S, but feed and product compositions and conditions are input, and the relative volatilities are calculated internally using the SRK equation of state. Distil2 contains a component library of over 400 components.

Distil-R - Rigorous distillation based on a Naphtali-Sandholm simultaneous correction method. Several K-value correlation are available, as well as a user supplied option. Contains a database with over 400 components.

Amine-1 - This program can be used for the preliminary design of plants for acid gas removal via amine absorption. Output includes a design summary with acid gas loading and removal rates, stream rates, and physical properties.

Mol sieve - This program sizes adsorber/regenerators of a gas dehydrator plant, based on 4A molecular sieves. Input requires a gas flow rate, feed composition, operating and design conditions. Output is bed diameter, bed pressure drop, bed height, and more.

PACKTWR - This program calculates the diameter and pressure drop of packed towers.

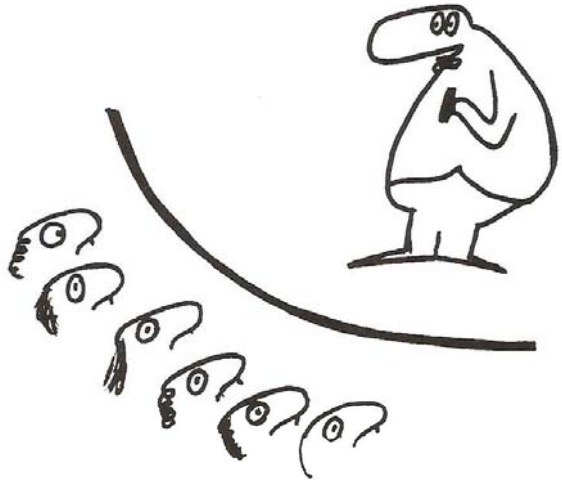
SWS1 - This program calculates the number of trays required for ammonia and hydrogen sulfide reduction in sour water stripping. A rigorous stage-to-stage calculation is performed.

VALTRAYG - This program designs and rates valve trays of up to 5 passes.

PROCHEM

ProChem is a specialized simulator that models interphase equilibria between aqueous-liquid, organic-liquid, vapor, and solids, interphase equilibrium (including Redox) and speciation, reaction kinetics, ion exchange and other adsorption processes. ProChem is offered by OLI Systems, Inc. (Florham Park, New Jersey).

Some applications of Prochem include simulations of amino acid separation by ion exchange chromatography, design of membrane separation processes, and simulation of gas treating systems using aqueous alkanolamine solutions.



Do NOT use this product for any purpose.
It might do something.

Microcomputer Chemical Engineering Programs (develped by 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 Professor Finlayson, nor will they be certified by CACHE.

In order to edit the column efficiently, the submissions must be made to Finlayson via BITNET, address FINLAYSON@MAX or on a diskette in ASCII. He will acknowledge receipt of the submission via BITNET and will send the edited column to the CACHE office via BITNET. Letters cannot be accepted.

The column can only be successful if professors submit their writeups. Let us hear from you!

REACT! A CHEMICAL EQUILIBRIUM CALCULATOR

By James A. O'Brien
Yale University

REACT! calculates chemical reaction equilibria by minimizing the Gibbs free energy of the reacting mixture, subject to conservation of material. It requires Microsoft(R) Windows 3.0 and at least 420k of free memory at startup. It is entirely menu driven.

Chemicals and initial mole numbers are chosen from a list, and initial temperature and pressure are selected through dialog boxes. REACT! then solves for the equilibrium mole numbers. In addition, REACT! can calculate and display a set of independent chemical reactions for the mixture of chemicals and an equilibrium constant for each reaction. Options are provided for adiabatic and/or constant volume reaction equilibria, in addition to the more standard isothermal isobaric conditions. The current version assumes immiscible solids and ideal gases. Thermodynamic information is built in for 90 chemicals (33 solids and 57 gases). REACT! is suitable for use in a ChE Thermodynamics or Reactor Design course.

For more information, contact:

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THERMAL DESIGN OF SHELL AND TUBE HEAT EXCHANGER

By Nurcan Bac and Ilker Ozal
Worcester Polytechnic

This program involves the thermal design of shell and tube heat exchangers conforming to TEMA specs. Propety data bank and physical property estimation routines for 243 chemicals are provided. Users have the ability to add or delete compounds. Physical properties of pure components, their mixtures and petroleum fractions are automatically generated. Some of the methods used in property estimation are outlined below:

Property	Method Used
Vapor heat capacity **Empirical Constants Reid et al. (1977)**	
Liquid heat capacity	**Bondi (1966)**
Vapor viscosity	**Stiel and Thodos (1962)**
Liquid viscosity	**van Velzen (1972)**
Vapor thermal conductivity	**Misic and Thodos (1961)**
Liquid thermal conductivity	**Reidel (1949)**
Latent heat of vaporization	**Pitzer (1955)**
Saturated vapor pressure	**Lee and Kessler (1975)**
Surface tension	**Brock and Bird (1955); Hakim (1971)**

User friendly, menu driven software asks for the following inputs:

1. Project name and title.
2. Fluids involved, and their locations. Shell and tube side flowrates and pressures.
3. Shell and tube inlet temperatures, and outlet temperature of one stream, or heat duty, or temperature approach.
4. Allowable pressure drops, fouling factors, initial overall coefficient estimate, initial geometry estimates (i.e. tube size, pitch, baffle spacing etc.) (Default values available).
5. Materials of construction.
6. Design pressures and TEMA class.
7. Chemical Engineering Plant Cost Index

The program performs Design or Rating tasks and optimizes the estimated fixed cost for the design case. The design mode also generates numerous alternatives with different geometry and cost. Summary screens indicate heat transfer and pressure drop details as well as cost estimates for plausible heat exchangers. Cost sorted lists and highly qualified specification sheets can be obtained for selected designs.

The program is developed during an M.S. thesis at METU Ankara, Turkey, and is useful in undergraduate heat transfer and design courses. The number of source lines are as follows : FORTRAN :4773, dBASE: 2853 , DOS (batch): 131 ; a total of 7757. The program runs on PC XT/AT or compatibles and on 386 machines. MS-DOS 2.0 or higher and minimum 320 kB RAM is required.Display is either monochrome or color. The program comes in a 1.2 MB 5.25 in. disk , or two 360 kB disks with password protection, a user's guide, and a sample problem. A disk can be obtained for a donation of $ 22.00 by writing to:

Professor Nurcan Bac
Chemical Engineering Department
Worcester PolytechnicInstitute
Worcester, MA 01609.

OPTIMUM SERIES BIOREACTOR DESIGN

By Gordon Hill
University of Saskatchewan

This program computes the "best" possible design configuration for series bioreactors to achieve any desired substrate conversion. It is based on optimization theory and presently permits the user to choose one of four possible bio-growth models: i)substrate saturation (Monod), ii)substrate inhibition (Haldane), iii)product inhibition I (Aiba hyberbolic) or iv)product inhibition II (Ghose linear). The calculations are used in biochemical engineering courses and in process design projects which utilize continuous bioreactors.

The user of the program provides biokinetic and feed stream information in an input file. This includes the type of growth model, the maximum specific growth rate, yields, saturation constant, inhibition constant, feed concentration and

final desired concentration. The program then evaluates the design strategy for a single CST bioreactor and the best design strategy for 2 series bioreactors. The user can then choose a final configuration (up to 10 series bioreactors). Typically, optimum designed bioreactors result in total processing volumes being decreased by factors ranging from 3 to 20 over a single CST bioreactor. In process design projects, this results in a significant drop in capital investment. Output is tabular in format and is sent to both the screen and to an output disk file.

The program is written in Turbo-Pascal and is provided in both source code and a math co-processor compiled version. A sample input data file and the corresponding best design strategy output file are also provided. A disk and descriptive information can be obtained for $12.00 (cheques payable to "University of Saskatchewan") by writing to: Professor Gordon Hill, Dept. of Chemical Engineering, University of Saskatchewan, SASKATOON, Sask. S7N 0W0, CANADA. Specify 3.5" or 5.25" & HD or MD.

The following programs have been listed in prior editions of the CACHE News.

1. Vapor compression refrigeration cycle, No. 24 and 25 Stanley Sandler, University of Delaware

2. Compression of an ideal gas, No. 24 and 25, Stanley Sandler, University of Delaware

3. Computer Aided Analysis for Process Systems, No.24 and 25, Ted Cadman, University of Maryland

4. Discounted Cash Flow Analysis (and Present Worth), No. 24 and 25, Bruce A. Finlayson, University of Washington

5. Short-cut Distillation and Flash Calculations, No. 24 and 25, Bruce A. Finlayson, University of Washington

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

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

8. Educational Software for Teaching Process Dynamics and Control, No. 26 and 27, Patrick Richard and Jules Thibault, Laval University

9. MIDAS - Microcomputer Integrated Distillation Sequences, No. 26 and 27, Andrew Hrymak, McMaster University

10. A Rigorous Multicomponent Multistage Steady-State Distillation Rating Program, No. 27 and 28, E.C. Roche, Jr., New Jersey Institute of Technology

11. RESIM. A Reactor Design Teaching Tool, No. 27 and 28, B.W. Wojciechowski, Queen's University

12. Real-time Multiloop Computer Control Program, UC ONLINE , No. 27 and 28, by Alan Foss, University of California at Berkeley

13. Real-time Dynamic Distillation Simulation and Relative Gain Program , No. 27 and 28, by Alan Foss , University of California, Berkeley

14. The Kinetics and Selectivity of Consecutive Reactions, No. 29 and 30, by Alvin H. Weiss and Reynold Dodson, Worcester Polytechnic Institute.

15. Equations of State, No. 30 and 31, by Kenneth R. Jolls, Iowa State University.

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CACHE Process Design Case Study Vol. 4
Alternative Fermentation Processes for Ethanol Production

The objective of this case study is the preliminary technical and economic evaluation of a fermentation process for the production of ethanol from a molasses feedstock. The intent is to expose the student to some non-traditional chemical engineering processes and to the rapidly expanding field of biotechnology. Groups of 2-3 students should be able to complete the design in about 30 days. The major focus of this design study is the creation and rational development of a suitable process flowsheet, simulation of the flowsheet by a commercial process simulator (in this case FLOWTRAN), and economic evaluation and cost minimization of the final process.

The problem begins with the specification of the plant operating requirements. The type of fermentor to be used as well as plant operating conditions are left open. Suggested fermentors include batch, CSTR, CSTR with cell recycle as well as a novel extractive fermentor based on the use of hollow fiber membranes, the Hollow Fiber Extractive Fermentor (HFEF). The choice of fermentor will affect the nature of the flowsheet and lead to several design alternatives. Given the time constraints, the student will have to rationally screen these alternatives before arriving at a workable flowsheet ready for simulation. A kinetic expression describing the production of ethanol from glucose is provided as well as a 5 1/4" floppy disk (IBM format) with a BASIC program for evaluating the performance of the CSTR fermentors. Performance characteristics are also provided for the batch fermentor and the HFEF. Detailed explanations and graphics are included to explain the results and the FLOWTRAN program for the suggested design.

The problem statement was posed by Professors Steven E. LeBlanc and Ronald L. Fournier and prepared under their supervision, by Mr. Samer F. Naser, all of the University of Toledo.

CACHE PROCESS DESIGN CASE STUDY VOLUME 4
"Alternative Fermentation Processes for Ethanol Production"

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CACHE Process Design Case Study Vol. 5
Retrofit of a Heat Exchanger Network and Design of a Multiproduct Batch Plant

This volume contains two short design projects that can be developed by groups of 2-3 students in about two weeks. As opposed to the large projects that are commonly used in a design course, the objective of the case study is to expose students to a greater variety of problems and which are of current industrial significance.

The first problem deals with the retrofit of a heat exchanger network consisting of 8 exchangers with 5 hot and 3 cold processing streams as well as steam and cooling water. The layout of the network and areas of the exchangers are also given. The objective is to determine a retrofit design that can reduce the energy consumption within specified limits for the capital investment and payout times. This problem requires examination of alternatives for the level of energy recovery, matching of streams, addition of area, and removal or reassignment of existing exchangers and piping. This problem can be used to illustrate basic concepts of heat integration, as well as the application of computer software such as Target II, THEN, MAGNETS and RESHEX. The second design problem deals with the design of a batch processing plant that has to manufacture 4 different products, all of which require 5 similar processing steps (reaction, product recovery, purification, crystallization and centrifuge). An important aspect of this problem is that the production schedule and inventory must be anticipated at the design stage. Furthermore, this problem also requires analyzing alternatives for merging processing tasks into single units, and using parallel units with and without intermediate storage. The use of Gantt charts is emphasized to examine some of these alternatives. The case study also includes two sets of homework problems with solutions that can be used to provide the basic background for the two problems.

This case study has been prepared by the students Richard Koehler and Brenda Raich at Carnegie Mellon University under the supervision of Professor Grossmann who developed the problem statements and educational material.

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A SERIES OF MONOGRAPHS ON AI IN CHEMICAL ENGINEERING

A series of monographs have been and are being written for use as main or supplementary material in advanced undergraduate and graduate courses addressing the application of expert systems or as a working introduction to AI by practicing engineers. Three monographs in the series are available. The purpose of these first three monographs is to provide detailed discussions on the principles, ideas, techniques, methodologies and issues of AI as they apply to chemical engineering. Later monographs will address approaches to specific problems of direct interest to chemical engineers such as fault diagnosis, design, etc. Currently available are:

Volume I, "Knowledge-Based Systems in Process Engineering: An Overview", is authored by George Stephanopoulos of MIT. This volume serves as an introduction to the monograph series and provides a broad perspective on AI. Specifically, this volume addresses the scope, history and market of AI and defines the need and role of knowledge-based systems in chemical engineering. Particular attention is paid to describing the general issues surrounding software and hardware environments.

Volume II, "Rule-Based Expert Systems in Chemical Engineering", is authored by James F. Davis and Murthy S. Gandikota of Ohio State University. This monograph focuses specifically on the implementation of knowledge-based systems in rule-based languages. The emphasis is not on the mechanics of rule-based programming environments, but on the issues which impact the implementation and performance of a system. While the focus is on rule-based implementations, many of the issues discussed cut across all general purpose implementation language. Using specific examples, the monograph covers these issues in detail. As a stand alone chapter, several of the most popular methods for various kinds of uncertainty handling are discussed and compared.

Volume III, "Knowledge Representation", is authored by Lyle Ungar of the University of Pennsylvania and V. Venkatasubramanian of Purdue University. The content of this monograph is directed at two distinct aspects of knowledge representation. In the first part of the monograph, the problem-independent issues and features of a variety of knowledge representations are presented. Included are discussions on semantic networks, frames, scripts and object-oriented programming. The second part addresses the subject of qualitative physics applied in chemical engineering. The issues of representing structure and behavior are discussed in detail. Examples demonstrating two philosophies are used to illustrate advantages and limitations.

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