CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

Vol. 26

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

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

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

For further information contact the Conference Chairman:

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

or Conference Vice Chairman:

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

Task Force: Artificial Intelligence in Chemical Engineering

Solicitation of Members for a Users' Group

CACHE is organizing a users' group with interests in artificial intelligence and computing technology (hardware and software). The goals of the users' group are to:

 Foster interaction among people with similar educational interests and needs.

ANNOUNCEMENTS

- b) Enhance exchange of software developed by the members of the group.
- c) Obtain group rates for commercial software.
- Develop a network with electronic mail and experimental bulletin boards for educational purposes.

To become a member of the users' group, write to:

Prof. George Stephanopoulos
Laboratory for Intelligent Systems in
Process Engineering
Dept. of Chemical Engineering
Massachusetts Institute of Technology
Room 66-562
Cambridge, MA 02139

Task Force: Artificial Intelligence in Chemical Engineering

Solicitation of Proposals for Case Studies on Expert Systems in Chemical Engineering

Proposals are solicited for the development and publication of Case Studies of Expert Systems Applications in the following areas:

- a) Diagnosis of Process Faults.
- Planning, Scheduling, or Maintenance of Process Operations.
- Design of Units, Processes, Controllers, Products, or Materials.
- d) Real-time Control Systems.

These approved case studies will be published by CACHE and will be distributed to all subscribing chemical engineering departments.

Submit proposals to:

Prof. George Stephanopoulos
Laboratory for Intelligent Systems in
Process Engineering
Dept. of Chemical Engineering
Massachusetts Institute of Technology
Room 66-562
Cambridge, MA 02139

BOOK REVIEW

An Introduction of Numerical Methods for Chemical Engineers, by James B. Riggs

This book is designed explicitly to provide undergraduates with the software and experience necessary to solve relevant chemical engineering problems. Of the more than seventy examples presented, approximately half pertain to chemical engineering, covering a wide variety of subspecialty areas. Although upper-division material is included in the examples, the more complex equations needed to solve these problems are derived in the text so that a student needs only to solve the resulting basic equations. Consequently, a student is exposed to a variety of chemical engineering numerical methods without needing a command of upper-division material. The book's emphasis is on solving algebraic equations (linear and nonlinear), initial value problems, and boundary problems. In addition, there is a chapter on optimization and one on process modeling.

An extensive collection of fully-documented, easy-to-use FORTRAN software for IBM-compatible PCs is included with the text. Equivalent software is available for Apple computers or mainframes. Library routines included with the software are: a linear equation solver, a multidimensional unconstrained optimizer, a variable step size/variable order integrator for ODEs, a finite element program, and a least squares, variable order spline data smoother.

In addition, a number of useful codes are developed in the text: a cubic spline interpolator, Thomas method, Gauss-Seidel method, N-dimensional Newton method, a Runge-Kutta integrator, a one-dimensional boundary value problem solver, a one-dimensional optimizer, a linear regressional method, a multiple linear regression method, an arc length homotopy algo-

rithm, and nonisothermal catalyst particle and fixed-bed reactor models.

The book is priced at \$45 (cloth) from Texas Tech University Press, Sales Office, Lubbock, Texas 79409-1037, USA, phone (800) 832-4042.

ANNOUNCEMENT OF CHEME-L LISTSERV

CHEME-L is a bulletin board/conference set of files that can be read and/or automatically distributed to your site. Current databases include the following:

An open forum.

"Is chemical engineering in crisis? Readying for tomorrow.

Evaluating the AIChE. Proposed improvements. (Opinions may be anonymous at the wish of the author. The survey will be submitted to the AIChE Council.)

You can contribute opinions by sending mail or files to CHEME-L:

sendfile filename CHEME-L at PSUVM

(The sendfile command is IBM VM/SP specific. Other systems may require another command.)

Research Collaboration Opportunities: This database collects information regarding requests for research collaboration and offers for research collaboration. To request the database send mail to r0mira01 at ulkyvm, with a simple message: "please send research collaboration file."

Chemical Engineering Education: You can contribute information of current interest such as: new trends or techniques, laboratory experiments, pointers to trend-setter articles on research or education (also a good way to advertise your own paper), unpublicized conferences or symposia, statistical data of interest to educators, etc. Send contributions to CHEME-L at PSUVM.

You can request this database by sending mail to r0mira01 at ulkyvm, with a simple message: "please send me chemical engineering education file."

Post-Doctoral Opportunities: This database

contains reference to post-doctoral openings and candidates. Contribute to it by electronic mail to CHEME-L at PSUVM.

Request this database by sending mail to rOmira01 at ulkyvm, with the message: "please send me postdoc search file."

Chemical Engineering Software: This database collects information about software. To contribute, send mail or a file to CHEME-L at PSUVM. Request the database by sending mail to r0mira01 at ulkyvm, with the message: "please send me chemical engineering software file." Note: This database collects only the references to the program; the actual programs are held at the authors' sites.

Chemical Engineering Funding: Request this database by sending mail to r0mira01 at ulkyvm, with a simple message: "please send me chemical engineering funding file."

Directory of Chemical Engineers: This database builds up automatically, and it will be distributed bimonthly beginning in March 1988.

CHEME-L Listserver was established by Raul Miranda of the University of Louisville. To subscribe to the listserver directly, send the appropriate interactive message:

To subscribe from an IBM VM/SP node:

TELL LISTSERV AT PSUVM SUB-SCRIBE CHEME-L your name

To subscribe from a VAX/VMS node:

SEND LISTSERV@PSUVM SUBSCRIBE CHEME-L your name SEND/FILE filename CHEME-L@PSUVM (MAIL command is available at some installations.)

To send opinions to be distributed or requests (from IBM):

NOTE CHEME-L AT PSUVM (write your letter, press the pF key to send mail)

or edit a file and send it:

SENDFILE filename CHEME-L AT PSUVM

A file with more information will be sent to you by listserve after subscribing.

CACHE Anthology of On-Line Computer Applications

The CACHE Anthology of On-Line Computer Applications in the Undergraduate Chemical Engineering Laboratory is now in the final stages of preparation. Publication is foreseen by the end of May.

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

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

The use of computers in the laboratory should be to enhance the student's learning experience. Much of the drudgery often associated with undergraduate laboratory work can be eliminated. In its place the student can be given the opportunity to interact easily with the experiment through the computer and with data taken by the computer. The object should be to let the student apply analysis at a higher level, and not to entirely replace analysis in the laboratory procedure. Some of the systems described in this volume have achieved this goal better than others, but all describe ways to revitalize and strengthen the laboratory experience.

Additional information can be obtained from either of the volume editors:

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

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

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

SOFTWARE FOR UNDERGRADUATE AND GRADUATE PROCESS CONTROL

by T. F. Edgar, The University of Texas at Austin

Linear system analysis has been the keystone of undergraduate control education for over 40 years. However, the growing availability of good, interactive software for controller design is causing some re-evaluation of the previous emphasis on analysis tools. At the same time, the coverage of the field of process control has been expanding; hence, there is pressure to eliminate or compress certain topics to make room for new material.

The historical dependence on Laplace transforms arose out of necessity because computational and graphical tools were not available. Rigorous analysis was necessary to obtain transient responses. This is not to say that one does not need to understand analytical responses for simple dynamic systems; but as a tool for complex systems, Laplace transform analysis is of marginal utility, especially when time delays exist in the process. In addition, when a PID controller is interfaced with a dynamic process, Laplace transforms are not a recommended approach to obtain the closed-loop response. It seems that the key to reducing the current course effort on linear systems analysis is good, interactive software. This will enable the instructor to cover other topics of current interest, such as batch control, safety analysis, statistical process control, artificial intelligence,

and the like.

The table entitled "Professional Software for Process Control" lists computer programs for general purpose controller design that have been discussed in the literature or for which there is advertising literature available at technical meetings. CACHE would like to survey those in chemical engineering who use these various software packages.

If you have experience with any of the programs listed in the table, please write to Prof. T. F. Edgar, Department of Chemical Engineering, University of Texas, Austin, Texas 78712. We hope to develop a list of experienced users for these programs so that up-to-date advice on software selection can be made available to faculty who teach process control.

In the table we have omitted such special purpose software as ACS (Advanced Control System from IBM) and UC-Online (Dr. Alan Foss, UC—Berkeley) because they are oriented towards specific multi-loop nonlinear processes such as a furnace or a distillation column. However, if there is any interest, information can be collected on such programs. There is already an ACS Users' Group formed to exchange information among faculty utilizing this software.

Professional Software for Process Control			
Program	Source	Features	Price (US \$)
CLADP, also Control System Toolbox with MATLAB	Cambridge Control High Cross Madingby Road Cambridge, England	PC or workstation. Controller design using pole/zero evaluation, matrix manipulation, Bode plots, Nichols charts, root locus, s-, z-, w- domains. Frequency response and state space methods for multivariable controllers. Icon-based version available for block diagrams (SIMBOL).	ask
CYPROS	Computer-Aided Modelling A/S N-7041 Trondheim Norway	Analysis of dynamic systems (statistical analysis, power spectra filtering, identification), parameter estimation and Kalman filtering, simulation of continuous or discrete and stochastic systems, optimal multivariable control, adaptive control, block-oriented simulation.	ask

Professional Software for Process Control			
Program	Source	Features	Price (US \$)
CC	Systems Technology, Inc. 13766 S. Hawthorne Blvd. Hawthorne, CA 90250-7083	PC-based, single loops, time and z-domain, frequency domain, root locus.	\$3,500 professional, \$1,100 aca- demic (10 copies)
CTRL-C	Systems Control Technology 1801 Page Mill Road P.O. Box 10180 Palo Alto, CA 94303-0888	Mainframe or workstation, matrix analysis, multivariable control, utilizes MATLAB, LINPAK and EISPACK, state space and frequency domain analysis.	ask
PC-PARSEL	Investment Soc. of America P.O. Box 12277 Research Triangle Park NC 27709	PC software, up to third-order transfer functions, optimum PID controllers, time and frequency domain analysis.	\$450
MATRIX-X	Integrated Systems 151 University Avenue Palo Alto, CA 94301	Mainframe or workstation, successor to MATLAB, provides classical or modern control tools, continuous or discrete time, adaptive control, signal processing.	\$8,000
Process Plus 3.0	Gerry Engineering Systems 13310 W. Red Coat Center Lockport, IL 60441	PID loop simulator of PCs, provides ten different industrial control algorithms plus Dahlin's controller, robustness plots, Bode plots.	
CONSYD	Prof. Harmon Ray Dept. of Chemical Eng. Univ. of Wisconsin Madison, WI 53706	Mainframe-based multivariable control, all domains, modeling and identification.	
ROBEX	Prof. Manfred Morari Dept. of Chemical Eng. Cal Tech Pasadena, CA 91125	PC-based for SISO design, user-friendly for a wide range of skill levels, designs robust PID/IMC controllers.	ask
TUTSIM, also DALS	Applied i 200 California Ave. #214 Palo Alto, CA 94306	PC program suitable for analog, digital and nonlinear control. Uses block diagrams or bond graphs to implement system equations term by term. Operating characteristics of the model are displayed graphically. \$300-\$ professi \$30 stu	
PROCOSP	D. R. Lewin Dept. of Chemical Eng. Technion-Isreal Inst. of Technology Haifa 32000 Israel	PC interactive system for PIC control. ask	
SIM TUNE	CHC Systems P.O. Box 61114 Phoenix, AZ 85082-1114	PC-based, simple models, valve and transmitter characteristics, PID controllers, tuning diagnostics.	\$850
KEDDC	Ingenieurbuero Erbele Jahnstr. 73 D-7441 Grossbettlingen FR Germany	Handles SISI of MIMO design using either classical or modern tools, time or frequency domain. Includes a variety of system identification methods, continuous or discrete controller design. Performs block-oriented continuous time simulation. Also designs adaptive controllers.	\$500-\$1,000 depending on system size.

NEW OPTIMIZATION FEATURE FOR FLOWTRAN

by J. D. Seader

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

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

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

> SCOPT, 34,885 bytes OPT8, 41,003 bytes OPSOL, 164,140 bytes

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

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

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

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

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

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

MICROCOMPUTER CHEMICAL ENGINEERING PROGRAMS

(developed by chemical engineering professors)



edited by Bruce A. Finlayson, University of Washington

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

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

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

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

Educational Software for Teaching Process Dynamics and Control

by Patrick Richard and Jules Thibault

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

can easily be changed within the program.

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

MIDAS—Microcomputer Integrated Distillation Sequences

by Andrew Hrymak, McMaster University

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

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

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

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

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

Convective Diffusion Equation (CDEQN)

by Bruce A. Finlayson, University of Washington

Program CDEQN solves a partial differential equation using either the finite difference method or the Galerkin finite method. The equation solved in CDEQN is the convective diffusion equation:

$$\frac{\partial x}{\partial t} + Pe \frac{\partial c}{\partial x} = \frac{\partial^2 c}{\partial x^2}, \ 0 \le x \le x_L \le 2.$$

The initial conditions are c(x,0) = f(x), where the function is set using the initial condition options in the program. The boundary conditions are

$$c(0,t)=c_0, \frac{\partial c}{\partial x}(x_L,t)=0.$$

The diffusion term can be left out to obtain the advection equation, and the convection term can be left out to obtain the diffusion equation. The integration in time is with a first-order Euler method. Options include solving for the spatial dependence with either the Galerkin finite element or finite difference method. Upstream weighting can be included or not as you wish. The results are plotted in the program ENGNPLOT (included). It runs on a Macintosh using pull-down menus. A sample result is shown.

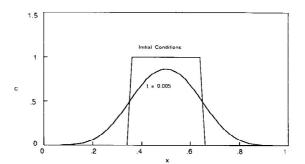


Fig. 1: Diffusion of concentration square wave.

This program has been used in a numerical analysis course, but is suitable for undergraduate heat and mass transfer courses. It runs on the Macintosh with 512K memory. The diskette with the system and the program on it requires an 800K drive, but the program itself fits on a 400K drive. A disk containing this program may be purchased for \$10, payable to Bruce A. Finlayson. Send requests to: Bruce A. Finlayson, 6315 22nd Avenue NE, Seattle, Washington 98115. The compiled program may be copied.

Engineering Plot (ENGNPLOT)

by Bruce A. Finlayson, University of Washington

The program ENGNPLOT is designed to make plots easily on command of the user. The program responds to either pull-down menus or typed commands. Basically the user enters the data to be plotted and the plot is made. The form of interpolation is linear between data points. The user can control the scale (log or linear), the

range of the graph, the number of subdivisions, the titles, the number of lines drawn, the use of symbols and connecting lines. Up to twelve captions can be placed anywhere on the graph. These captions can use several fonts, boldface, underlines, etc. The data can be read from a file or entered from the keyboard. The plots can be printed or saved as a screen image; this can then be put into MacPaint, and hence into any Macintosh document. A sample plot is shown.

The program can be used in a stand-alone fashion in courses such as laboratory. It is used as the plotting package for other programs mentioned in this issue and has been thus used by many students in different courses.

The program runs on the Macintosh with 512K memory. The diskette with the system and the program on it requires an 800K drive, but the program itself fits on a 400K drive. A disk containing this program may be purchased for \$10, payable to Bruce A. Finlayson. Send requests to: Bruce A. Finlayson, 6315 22nd Avenue NE, Scattle, Washington 98115. The compiled program can be copied.

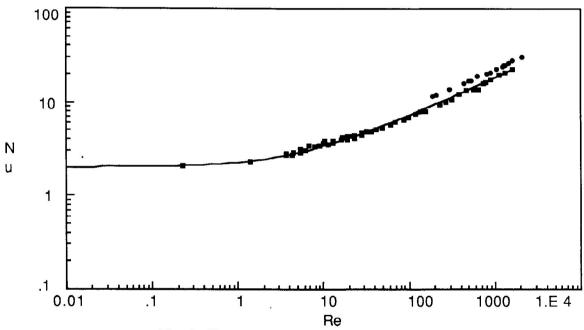


Fig. 2: Nusselt number for air at low delta t.

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

To: Grand@LSUCHE
From: person id@node id
help

- (1) Vapor Compression Refrigeration Cycle & Compression of an Ideal Gas, by Stanley Sandler, University of Delaware
- (2) Computer-Aided Analysis for Process Systems, by Ted Cadman, University of Maryland
- (3) Discounted Cash Flow Analysis (and Present Worth), by Bruce A. Finlayson, University of Washington Short-cut Distillation and Flash Calculations, by Bruce A. Finlayson, University of Washington

CURRICULUM TASK FORCE

CACHE IBM PC Lessons for Chemical Engineering Courses Other Than Design & Control

The Curriculum Task Force of the CACHE Corporation is completing the experimental phase of its project to prepare computer-based lessons for chemical engineering courses other than design and control. These lessons are intended to expose the students to "open-ended" problems and typical design alternatives. In the Fall of 1987, departments that support CACHE received a complimentary set of the six lessons on separate

diskettes. The table summarizes the lessons that were included

Departments that do not support CACHE may purchase each lesson individually for \$25 per lesson.

All of the lessons run on the IBM PC and may be installed on a shared network. Copies of the diskettes may be made for distribution to classes of students.

	CACHE IBM PC Lessons			
Lesson (Program)	Authors	Applicable for Courses in		
Slurry Flow in Channels	B. Freeman, W. Provine, G. Dow & M. M. Denn, Berkeley.	Fluid Mechanics		
Supercritical Fluid Extraction	J. Kellow, M. L. Cygnarowicz & W. D. Seider.	Separations and Thermodynamics		
Gas Absorption with Chemical Reaction	K. Nordstrom & J. H. Seinfeld, Cal. Tech.	Separations		
Design of Flash Vessels and				
Distillation Towers	B. A. Finlayson, E. W. Kaler & W. J. Heideger, Washington.	Separations and Thermodynamics		
Heterogeneous Reaction Kinetics	J. E. Bauer & H. S. Fogler, Michigan.	Reactor Analysis		
CSTR Dynamics and Stability	L. E. Vajdi & D. T. Allen, UCLA.	Reactor Analysis		

Fluid Mechanics Course

The Curriculum Task Force of the CACHE Corporation is beginning Phase II of its project to prepare computer-based lessons for chemical engineering courses other than design and control. The focus will be upon the fluid mechanics course, a course in which the computer has not been used actively. Two projects are being initiated and are described below.

Project to Prepare IBM PC Lessons

Two authors, Prof. Mark McCready of Notre Dame and Prof. Deniz Karman of New Brunseich), have begun to develop a set of lessons. Prof. McCready will focus on the laminar flow of liquids in simple geometries and Prof. Karman will emphasize the matching of pump and pipeline characteristics, pipe networks, and other topics. Others are welcome to participate, and should contact:

Prof. Warren D. Seider University of Pennsylvania Department of Chemical Engineering Towne Building 220 South 33rd Street Philadelphia, Pennsylvania 19104-6396 CACHE is providing the authors with copies of the UNISON Authoring System (Courseware Applications, Inc.). UNISON was judged by the Curriculum Task Force as best-suited for the preparation of this next generation of lessons. It has excellent facilities for the preparation of tutorial materials (including text, questions and graphics) and greatly simplifies the preparation of annotated graphics displays which will be particularly important for the lessons in fluid mechanics. With UNISON, it should be possible to present the technical concepts using animation in a way that textbooks cannot accomplish.

Project to Develop Lessons Using Advanced Workstations

The curriculum Task Force is soliciting proposals to develop a lesson(s) using workstations that are more advanced than the IBM PC. We envision a lesson(s) involving the simulation of flows through irregular conduits, possibly with free surfaces. Such lessons would require high-

resolution graphics and a reasonable amount of computing speed and storage to perform the finite element analysis—rather, they would perform experiments with the simulator, trying different configurations, calculating power requirements, etc.

Ideal authors are those performing research in this area. These persons could easily assemble several of their less experimental programs for use by the undergraduates. Persons working on research involving the numerical methods, or studying unusual flow (eg., through heart valves, etc.) would be ideally suited to participate.

If you are interested in the project, please contact:

Prof. John H. Seinfeld Chemical Engineering, 206-41 California Institute of Technology Pasadena, California 91125 (818) 356-4635

ARTIFICIAL INTELLIGENCE TASK FORCE

A Series of Monographs on Knowledge-Based Systems in Process Engineering

by George Stephanopoulos

The CACHE task force on Artificial Intelligence in Process Engineering has launched a project leading to the development of a series of monographs on the subject of "Knowledge Based Systems in Process Engineering." The purpose of these monographs is to provide an educational vehicle in this new exciting area. They are intended as main or supplementary material in advanced undergraduate or graduate courses in chemical engineering curricula, or as introductory reading to this area by practicing engineers at large.

The series of monographs will be composed of the following volumes:

- I. Knowledge-Based Systems in Process Engineering: An Overview
- II. Rule-Based Expert Systems
- III. Advanced Knowledge Representation & Control
- IV. KBES for Process Fault Diagnosis
- V. KBES for Planning & Scheduling Process Operations
- VI. KBES for Process Control
- VII. KBES for Engineering Design

The first three volumes have already been under development and should be available from CACHE in early September 1988. The remaining four volumes are expected to be out by Spring 1989.

Volume I, authored by George Stephanopoulos of MIT contains the following:

Chapter 1: Introduction to the Series of Monographs

Chapter 2: What is AI?

The scope of AI
A brief history
The market of AI

Chapter 3: Knowledge-Based Systems

Why are they needed?

KB systems in chemical and biochemical engineering

Modeling, modeling, modeling

Chapter 4: KB Systems & Programming Environments

Data-driven vs. procedural programming
The notion of object-oriented programming

Symbolic computing

Software support for KB systems' development

Computer hardware

Chapter 5: Summary & Conclusions

Volume II is being developed by M. S. Gandikota and J. F. Davis of Ohio State University. It contains the following material:

Chapter 1: Understanding Rule-Based Expert Systems

Overview Motivation

Working definition

Outline of the monograph

Chapter 2: Rule-Based Languages Contrasted with Conventional Computational

Languages

Comparison at the processing level

Comparison of the problem characteristics Comparison of knowledge representation

Chapter 3: Knowledge Representation

Purpose of knowledge representation

Types of expert knowledge

Knowledge representation schemes Knowledge representation in rules

Analysis

Chapter 4: Reasoning & Control

Reasoning strategies
Control strategies

Analysis

Chapter 5: Architecture of Rule-Based Systems

Chapter 6:

Uncertainty Handling

Uncertain data and/or knowledge Representation of Uncertainty

Chapter 7:

Development of a Rule-Based Expert System: A Complete Chemical

Engineering Example

Identification
Conceptualization
Formalization
Implementation

Testing

Volume III is being developed by L. Ungar of the University of Pennsylvania and V. Venkatsubramanian of Columbia University. Its contains the following:

Chapter 1:

Semantic Nets & Frames

Limitations of rule-based representations

Types of knowledge to represent

Semantic nets

Frames

Comparisons & examples

Chapter 2:

Objects & Object Relationships

Objects, the basis of modeling

Role of objects in structuring knowledge

Rules vs. objects

Object-oriented programming

Message passing

Chapter 3:

Scripts

Roles, props, actors, scripts

Triggers, necessary and optional events, user-initiated events

Chapter 4:

Qualitative Physics

Why?

Speed, generality

Order-of-magnitude reasoning Device-centered ontologies

Chapter 5:

Constraint Propagation

Definitions, examples Truth maintenance Multiple worlds

Chapter 6:

Problem Structure & Control of Reasoning

Structure of Problems

Goal-driven vs. data-driven reasoning

Higher-level structures
Blackboard architectures

DESIGN CASE STUDIES TASK FORCE

by Manfred Morari & Ignacio Grossman

As a result of the call for proposals last year, two new case studies are under development

Profs. Le Blanc and Fournier at the University of Toledo are developing a case study is entitled Alternative Fermentation Processes for Ethanol Production-Preliminary Design and Economic Analysis. This project deals with the integration of a process flowsheet where a number of alternative fermentors are considered. The case study will include a floppy disk for the simulation of the fermentors. Also, it shows how the fermentaprocess can be simulated FLOWTRAN. This case study should be completed this summer and ready for distribution in the fall.

The other case study is being developed by Professor Ed Roche at the New Jersey Institute of Technology, with the collaboration of Exxon Research and Engineering. The case study is entitled *Design of a Gas Oil Hydrodesulfurization Unit*. This case study illustrates the use of pseudo components for handling complex hydrocarbon mixtures. The problem involves the reactor design, selection of separation technologies and heat integration. Simulations are performed with PROCESS and DESIGN 2000. It is expected that this case study will be completed this summer.

Enclosed with this newsletter you will find a call for proposals for CACHE Design Case Studies. We encourage faculty teaching undergraduate design courses to submit proposals if they have design projects that are compatible with the educational goals of the Design Case Studies Task Force and the guidelines given in the call for papers. Proposals involving nontraditional chemical engineering tasks, e.g., semiconductor processing, bioprocessing and materials will be given preference. Retrofit design problems are also of great interest, and projects with industrial participation are viewed favorably. Funding up to \$5,000 is available for each project.

Finally, to get feedback on the first three design case studies that CACHE has produced, we will be sending a questionnaire within the

next few weeks. We will very much appreciate your response to the questionnaire.

CALL FOR PROPOSALS FOR THE PREPARATION OF CACHE PROCESS DESIGN CASE STUDIES

Over the last two years, the CACHE Process Design Case Study Task Force has published the following three case studies:

- 1) Separation System for Recovery of Ethylene and Light Products from a Naptha Pyrolysis Stream.
- 2) Design of an Ammonia Synthesis Plant.
- 3) Design of an Ethanol Dehydrogenation Plant.

These case studies, which were developed by member of the task force, have been well received. As a result, CACHE is seeking to expand the project to include high-quality contributions from our faculty colleagues at large. In fact, two new case studies are currently under preparation in response to our call for proposals in 1987.

We are seeking new proposals for the development of a CACHE Process Design Case Study and are willing to provide funds to a maximum of \$5,000. This money can be used, for example, to pay the stipend of an undergraduate/ graduate student, to contribute to the summer salary of the supervisor or to cover other office expenses.

Proposals involving nontraditional chemical engineering tasks, e.g., semiconductor processing, bioprocessing and materials will be given preference. Retrofit design problems are also of great interest, and projects with industrial participation are viewed favorably. Proposals should be directed to either of the following professors:

Prof. Manfred Morari Chemical Engineering 206-41 Caltech Pasadena, CA 91125 Prof. Ignacio E. Grossman Dept. of Chemical Engineering Carnegie Mellon University Pittsburgh, PA 15213

As a reminder, the goal of the Design Case Study Task Force is the development of case studies to aid process design education. Though no two design problems are alike, there is a general logical sequence of basic steps which lead to a good design. It is the chief objective of the

CACHE Case Studies to demonstrate and clucidate this thought and decision process. The CACHE Case Studies should be different from final student or industrial project reports in that they do not only present one final solution, but show the whole solution procedure leading from the problem statement to the final solution(s) in an organized manner. Within that philosophy, neither is the scope fixed nor the methodology limited. Eventually, a library of case studies is sought ranging from small ones to large ones and covering a variety of design aspects.

Status of GRAND Wide Area Network File Server at Louisiana State University

by Danny Reible and Peter Rony

The GRAND wide area network file server on the LSU Department of Chemical Engineering IBM is now operational. More details will be sent soon by Danny to all CACHE member departments. In the following, the experiences of a remote user, the second author at Virginia Tech, will be described. Tests were done during the evening on Sunday, March 20, 1988. GRAND responses were very rapid in view of the low traffic on the BITNET network at that time.

The remote user signed up on the GRAND system several months ago over the BITNET network using the IBM mainframe TELL command:

TELL GRAND AT LSUCHE SIGNUP PETER R. RONY

Alternatively, the MAIL command could have been used to send the following command to GRAND at LSUCHE:

SIGNUP PETER R. RONY

Several weeks later, help was requested:

TELL GRAND AT LSUCHE HELP

On March 20, 1988, the remote user requested to see the bulletin board subject areas:

TELL GRAND AT LSUCHE CONF CACHE GET CACHE DIRECTRY

Again, this request could have been sent via a MAIL message:

CONF CACHE
GET CACHE DIRECTRY

The CACHE DIRECTRY (not directory) file listed eleven INDEXES, which could be accessed by the following series of commands:

TELL GRAND AT LSUCHE CONF CACHE GET HELP INDEX

TELL GRAND AT LSUCHE CONF CACHE GET NEWSLETR INDEX

TELL GRAND AT LSUCHE CONF CACHE GET PROJECT INDEX

TELL GRAND AT LSUCHE CONF CACHE GET SOFTWARE INDEX

TELL GRAND AT LSUCHE CONF CACHE GET TELECONF INDEX

TELL GRAND AT LSUCHE CONF CACHE GET STUDENT INDEX

TELL GRAND AT LSUCHE CONF CACHE GET JOURNAL INDEX

TELL GRAND AT LSUCHE CONF CACHE GET FACULTY INDEX

TELL GRAND AT LSUCHE CONF CACHE GET CAST INDEX

TELL GRAND AT LSUCHE CONF CACHE GET ACS INDEX TELL GRAND AT LSUCHE CONF CACHE GET TEACHING INDEX

Six of these indexes contained the following files on March 20:

CHEME LISTSERV
NUMANAL LABS
CACHE NAMES
EMAIL REPORT
CAST MEETINGS
MARCH88 NEWSLETR
ACSESS NAMES
LSUACS MANUAL
ACS BLENDER
PURDUE MINUTES
ACS 88LA MEETING

These eleven files were retrieved by the remote user using the following GRAND commands:

TELL GRAND AT LSUCHE CONF CACHE GET CHEME LISTSERV
TELL GRAND AT LSUCHE CONF CACHE GET NUMANAL LABS
TELL GRAND AT LSUCHE CONF CACHE GET CACHE NAMES
TELL GRAND AT LSUCHE CONF CACHE GET EMAIL REPORT
TELL GRAND AT LSUCHE CONF CACHE GET CAST MEETINGS
TELL GRAND AT LSUCHE CONF CACHE GET MARCH88 NEWSLETR
TELL GRAND AT LSUCHE CONF CACHE GET ACSESS NAMES
TELL GRAND AT LSUCHE CONF CACHE GET LSUACS MANUAL
TELL GRAND AT LSUCHE CONF CACHE GET ACS BLENDER
TELL GRAND AT LSUCHE CONF CACHE GET PURDUE MINUTES
TELL GRAND AT LSUCHE CONF CACHE GET ACS 88LA MEETING

The JOIN command did not work for the remote user on March 20. The commands ADD and LEAVE were not tested. The authors hope that the above will stimulate the testing of the GRAND system during the next several months.

STANDARD LIST OF BITNET USERID NICKNAMES

by Peter R. Rony

I have started to develop a list of nicknames, in IBM/VM format, for chemical engineering colleagues throughout the world. A second draft (February 29, 1988) was available at the AIChE Meeting in New Orleans. It does not yet contain the userids of complete departments, for example, Maine, Utah, North Carolina State, Georgia Tech, LSU, and others.

The draft RONY NAMES A0 file is available for BITNET transmission to anyone who requests this file from me. It is immediately useful for IBM mainframes, as Ali Cinar at IIT has confirmed, but is not useful for VAX systems.

The use of nicknames means that you no longer need remember the userid or usernode at CACHE chemical engineering institutions. You can simply send a message to SMITH, JONES, ZABOTINSKII, and others through the IBM mainframe MAIL command,

MAIL JONES (file RONY NAMES A0)

or MAIL JONES

for example.

At the CACHE Trustees meeting in New Orleans, a proposal was made to standardize the BIT-NET nicknames for any type of computer. As the proposal stands at present:

- (a) For a unique last name in the chemical engineering international community, the last name is the total nickname.
- (b) For a non-unique last name, the first six characters of the last name followed by the first initial followed by an optional one-digit number is the total nickname. As an example, for Fred R. Zabotinskii and Frank E. Zabotinskii, the nicknames are, respectively, ZABOTIF0 and ZABOTIF1.
- (c) For a non-unique last name that has fewer than six characters, the full last name followed by the first initial followed by an optional one-digit number is the total nickname. As an example, for Ju Chin Wang and Ju Shu Wang, the nicknames are, respectively, WANGJ0 and WANGJ1.
- (d) The nicknames can be modified locally if desired. The idea is to save time for BITNET users by providing a starting NAMES file that can be tailored to local preferences. The nicknames only apply on the local BITNET node and are not broadcast as messages.
- (e) Initially, the nickname list will be handled and updated every two months by RONY at VTVM1. It will also be a file on the GRAND system at LSU.
- (f) Comments and suggestions concerning the nicknames should be sent to RONY at VTVM1.

What to do about VAX nicknames? Venkatesh Chittur (CHITTUR at PURCHE) provided the following comments on March 1, 1988: "For people who are on Unix systems, the equivalent thing to having a file like RONY NAMES would be to have a file called ".mailrc" in the home directory (this should be obvious to anyone familiar with Unix, so do not worry about it). This file will contain lines like

alias peter rony at vtvml.bitnet alias venky venky at purche.bitnet

and so forth. So, when I say "mail peter," it means "mail rony at vtvm1.bitnet."

"In fact, one can have lists too. For example,

alias people rony at vtvm1.bitnet chittur at purche.bitnet gvr at purche.bitnet

I can thus say "mail people" to mail a message to everyone in the alias people list. I am not certain if you are familiar with this capability, so I thought that I would mention it."

BITNET Network Information Center, EDUCOM

by Peter R. Rony

"We would very much like to access our colleagues in the various chemical engineering departments via the BITNET network, but we have been hampered by the lack of hard information as to how to access the system, as well as addressing codes at the various institutions." "We would like to know how we can participate in the BITNET user's program and cost associated with the service, including that for the software package, GRAND."

These are two quotes from colleagues overseas who wish to have active BITNET nodes at their institutions. In previous issues of *CACHE News*, we have described what BITNET is. In this issue, we wish to provide information on how to join BITNET, keep current with BITNET developments, and seek information that may not be available locally.

BITNET is governed by an incorporated Board of Trustees elected from its membership. Day-to-day operations and support are provided by the BITNET Network Information Center located at EDUCOM and funded by membership fees. The address of EDUCOM is P.O. Box 364, Princeton, New

Jersey 08540, (609) 520-3377. The BITNET userid and node is BITNET at BITNIC. You can access general information by sending a message to INFO at BITNIC.

I called Isabel Sellers in the networking section of EDUCOM and asked her to send me the typical package generally sent to an organization that wishes to join BITNET, and received the following documentation:

"Criteria for BITNET Membership" (5 pages)

"Procedures for Joining BITNET" (5 pages)

"Application for BITNET Membership" (3 pages)

"Required Site/Node Information" (5 pages)

"BITNET and the BITNIC: The BITNET Network Information Center at EDUCOM" (2 pages)

"MVS/BITNET: Possible Environments" (2 pages)

"Non-IBM BITNET Communications Support (Non-IBM Communications Environments with which RSCS Communicates)" (2 pages)

"BITNET Tools" (2 pages)

"RSCS Emulators Available" (2 pages)

"The Columbia University MAILER: A Mail Transport Server" (2 pages)

"BITNET: Past, Present, and Future," by Daniel J. Oberst and Sheldon B. Smith, EDUCOM Bulletin, Summer 1986.

"BITNET/EARN/NETNORTH Topology as of 7 February 1988" (25 pages)

"BITNET Institutional Representatives," BIREP LIST 2/88 (15 pages)

"BITNET Member Institutions," 02/17/88 (8 pages)

I am a regular recipient of EDUCOM literature, such as "EDUCOM Information Technology Seminars" and EDUCOM'87, an announcement of last year's conference dedicated "Toward a Global Information Culture: Education, Libraries, and Technology."

The following items from this package of literature caught my attention.

- (1) If a CACHE member wishes to know who the representative is at his or her institution, give me a call at (703) 961-7658 or send a message to RONY at VTVM1.
- (2) The same offer applies if you wish to know if your institution has a BITNET node, in which case I guess you will have to call.
- (3) I do not have lists of representatives or institutions of NETNORTH and EARN; the topology listing that I do possess lists institutions only by connection date and topology.
- (4) The general membership categories of BITNET are the following:

Class A: Certain degree-granting institutions of higher education.

Class B: Certain consortia and affiliates of institutions of higher education.

Class C: Certain nonprofit organizations serving higher education.

Class D: Certain governmental, commercial, industrial, or nonprofit organizations with substantial research or educational links to institutions of higher education.

Class E. Certain governmental, commercial, industrial, or nonprofit organizations with substantial research or educational links to institutions of higher education.

For further details, see "Criteria for BITNET Membership." Industrial members of BITNET include E. I. Du Pont de Nemours and Co., Inc., IBM Almaden Research Center, IBM VNET Gateway, Control Data Corporation, Exxon Research and Engineering Company, IBM Watson Scientific Research Center Yorktown, and Chemical Abstracts Service (American Chemical Society). Federal agencies that are members of BITNET include Food and Drug Administration, National Academy of Sciences, National Science Foundation, Smithsonian Institution, The World Bank, Argonne National Laboratory, Fermi National Accelerator Laboratory, National

Aeronautics and Space Administration, National Bureau of Standards, National Institutes of Health, United States Department of Agriculture, National Institute of Environmental Health Sciences, Los Alamos National Laboratory, Brookhaven National Laboratory, NASA Goddard Institute for Space Studies, and Oak Ridge National Laboratory. Two professional organizations that are BITNET members are the American Physical Society and the Association for Computing Machinery (ACM).

(5) "Non-IBM BITNET Communications Support" includes the following information:

Computer/System	Software
VAX 11/7xx under VMS	JNET (Joiner Associates)
VAX 8600 under VMS	JNET
MicroVAX II under VMS	JNET
VAX/Unix (Berkeley)	UREP (Penn State University)
VAX/Unix (Berkeley)	HOMEBREW, BERKHASP
DEC PDP 11/xx	UREP, HOMEBREW, BERKHASP
Sun-2/Unix	UREP
CDC Cyber under NOS	NJEF, AMF, MTF (Control Data Corp.)
Sperry 1100 under OS 1100	RTP/1100 (Sperry)
PRIME 750 and 950 under PRIMOS	PRIMENET

- (6) "Jnet allows users of VAX-11 and MicroVAX computers running VAX/VMS to exchange files, electronic mail, and real-time messages with users of IBM 370, 43xx, and 308x computers running under IBM's VM/SP with CMS, and other VAX/VMS systems running Jnet. Jnet enables VAX-11s and MicroVAXes to communicate over bisynchronous communication lines using IBM's RSCS (Remote Spooling Communications Subsystem) protocol. To IBM computers, an attached VAX system running Jnet appears to be another computer running VM/SP with full routing capabilities. Jnet provides VAX/VMS DCL (Digital Command Language) commands to send files, network commands, and messages over an RSCS network. Jnet also includes software that provides an interface between BITNET and DEC's VMSmail, the standard mail system that is included as part of VAX/VMS software." See "RSCS Emulators Available."
- (7) "At the Pennsylvania State University, a system is being developed under UNIX to emulate the functions of IBM's Remote Spooling Communications Subsystem (RSCS) network." See "RSCS Emulators Available."
- (8) File servers, now resident at many nodes on the network, automatically respond to user requests in the form of messages, mail, or files. File servers vary in the range of services and information provided. A file server being developed at LSU for the chemical engineering community is called GRAND. Representative servers on BITNET, EARN, and NetNorth include:

Server Name	Institution	Contents
CANSERVE	University of Guelph	General purpose files, topical notebooks that allow user addition.
CSNEWS	University of Maine	General information files, EXEC/REXX utilities, Maine's VM/COM newsletter, BITNET user lists.
DATABASE	BITNIC	BITNET NAMES file (node information) database, ARPANET digests, PATHFINDER database.
KERMSRV	Columbia University	KERMIT documentation and program files for micros and mainframes.

Server Name	Institution	Contents		
LFCNET	National University Computer Center Pia	REXX, VM/CMS, and BITNET topics: mathematical subroutines, provision for communication within academic discipline groups.		
MACSERVE	BITNIC	Public domain Apple Macintosh software.		
NETSERV	Gesellschaft fuer Schwerionen forshung Darmstadt	EARN documentation, node lists, topologies, user lists, software and software problem files.		
NICSERV	BITNIC	Gateway documents, BITNIC policy and facility documents, description of mail environments, technical working group communication records, EDUCOM NETWORKING newsletter.		
SERVER	University of Guelph	General information files and EXEC/REXX utilities.		
VMBBOARD	Weizmann Institute of Science	General interest files, user names, microcomputer information.		

(9) From "BITNET: Past, Present, and Future," a BITNET Applications Sampler:

"Yale University Press uses BITNET in many areas, including electronic mail dialogues with authors in all stages of publishing, often shipping complete manuscripts to editors. With two separate encyclopedia projects underway at remote locations, the Press uses BITNET to send a constant flow of articles to and from project editors and in-house manuscript editors. In addition, indexers employed by Yale at remote institutions receive manuscripts via BITNET, returning completed indexes the same way."

"EDUCOM professional and support staff use BITNET to keep in touch with conference and seminar speakers; to communicate with Board of Trustees members; to collect, edit, and ship meeting minutes; and to correspond with the EDUCOM Membership Committee for application approval. EDUCOM consultants ship and receive consulting reports via BITNET, and the HEDS project ships files to and from the central database at Cornell. For the 1985 conference, EDUCOM received 77 inquiries via electronic mail. The publications department also ships manuscripts to and from authors writing for the EDUCOM Bulletin and other publications."

"The Theoretical Chemist Research Group at the Cannata Research Computation Center (CRCC) and Andrew McCammon and Montgomery Pettitt exchange software over BITNET with research associates at the University of California at San Francisco, Purdue, Texas A&M, Harvard, and MIT. Papers and manuscripts are submitted to publishers via BITNET, and theoretical chemists working with Donald Kurt Kouri use BITNET to exchange manuscripts with European and Israeli research associates."

(10) An example of a required site/node IBM/VM entry is as follows:

nick VANVAX1
alias VANVAX1
via VANLONVM
net BITNET
site Vanlon University--Computational Sciences VAX1
system VMS 3.1
machine DEC VAX 11/750
netsoft jnet

nick VANVAX1

alias VANVAX1

via VANLONVM

net BITNET

site Vanlon University--Computational Sciences VAX1

system VMS 3.1

machine DEC VAX 11/750

netsoft inet

msgs YES

cmds YES

files YES

country USA

longitude 064W 022

latitude 045N 006

connect 03/28/87

mailer

postmast (Wanda Bestok) BESTOK at VANVAX1 (203) 555-1212

gates none

mformat PUNCH

mclass M

fformat PUNCH

flcass N

tformat PUNCH

tlcass A

bitdirector (Jane Blankowitz) BLANK at VANLONVM

inforep (Michael Jarter) JARTER AT VANVAX1

techrep (Horace Dibble) DIBBLE AST VANVAX1

contact (Martha Opperman) OPPIE AT VANVAX1

informl (Martha Opperman) OPPIE AT VANVAX1

infol jnet

linkfail (Technical Services) TCHSRV at VANVAX1

addr Computational Sciences Building

MS-333

Upper Harvonton, NY 01234

linkspeed 9600

linktype DECNET

Incidentally, the RONY NAMES A0 file (see article in this issue by Rony) has a similar form for each nickname entry:

nick.OCONNELL

userid.cykjycs

node.nervm

addr.University of Florida

STATUS OF FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

by J. D. Seader

As a part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to chemical engineering departments to install on their in-house computers. Thus departments would be able to run FLOWTRAN at no additional charge. CACHE continues to supervise the preparation of FLOWTRAN load modules for some mainframe. supermini, and supermicro-type digital computers and the distribution of the modules on magnetic tape to departments that order them. A new optimization feature is now included, and the instructional FLOWTRAN book is now in its third edition. Please see the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

DEC VAX computers running with the VMX operating system.

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

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

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

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

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

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

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

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

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

Honeywell computers with CP6 operating system.

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

University	Computer
Ohio State U.	DEC VAC 8500
U. of Tulsa	Honeywell T6600
Youngstown State U.	Amdahl 5868
U. of Iowa	Apollo DOMAIN
E. China U. Tech., Shanghai	DEC MicroVAX 11
Hampton U.	DEC VAX 11-780
U. of Pennsylvania	DEC VAX 8650
U. of Southern California	DEC VAX 11-750
Tsinghua U., China	DEC VAX 11-750
S. Dakota School of Mines	CYBER 830-180
U. of South Alabama	CRAY X-MP/2

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

LSU/CACHE BULLETIN BOARD GENERAL INFORMATION AND USER'S MANUAL

In cooperation with IBM, LSU is operating a bulletin board/teleconferencing system for the CACHE consortium of chemical engineering departments. The bulletin board will act as a central storehouse of information of interest to CACHE members that can be accessed through the BITNET electronic communications network. Faculty members who can send and receive electronic mail on BITNET can send or receive bulletin board information. The information on the bulletin board is segregated by subject; among the subjects that will be maintained are:

CACHE Newsletters
CACHE Projects
CAST (AIChE) Newsletters and Information
Contributed Public Domain Software
CACHE Faculty Electronic Mail Addresses
Prospective Graduate Student Addresses
IBM Advanced Control System Information
Teleconferences

The entire bulletin board will be supervised by the IBM/GRAND teleconferencing system on the LSU Chemical Engineering Department's central computing system. Among the advantages of using this system is that information can be accessed, retrieved or added to without operator intervention. In addition, a user can join a particular topic and GRAND will notify him or her whenever another user has added information to the topic. Another key advantage is the use of the free-to-the-user BITNET electronic mail network to which most campuses are attached either directly or indirectly through another network.

The purpose of this report is to solicit contributions and to acquaint interested faculty in the procedures for use of the system. It is recognized that the success of the bulletin board is totally dependent on the quality and quantity of its offerings and the ease with which they can be accessed and retrieved by users.

GETTING STARTED: Testing the electronic mail connection.

The LSU/CACHE Bulletin Board can be accessed in two ways: through primitive commands sent as messages or mail over BITNET, or

through an elaborate userfriendly menu-driven interface program called CONFER. Unfortunately, CONFER is only available for IBM computer systems employing the virtual machine operating system (VM). For those departments that use this operating system, it is expected that CONFER will soon be available from LSU. For other users, however, only five commands need be learned to use all of the basic capabilities of the bulletin board. These commands can be sent to the bulletin board using the BITNET message commands (e.g., TELL) or electronic mail using BITNET or another network (e.g., ARPANET).

To avoid confusion, let us assume that communication with the bulletin board will be via electronic mail that is invoked with a command MAIL. To send a command to the bulletin board from a BITNET site, type:

MAIL GRAND AT LSUCHE

Here the address contains the user ID of the bulletin board (GRAND) on the BITNET node LSUCHE (the LSU chemical engineering computer). The note that you are mailing should contain the single command HELP. If this note is sent, the bulletin board would respond with some general help information. Depending on the response time of the network, it may take several minutes or longer for the bulletin board to receive the message and respond. When the response is received, the file that the bulletin board sent can be received and reviewed using your system's editor or browse facilities. No special handling of the received file is necessary.

The help file will describe general usage of the conferencing system, including how to send commands interactively rather than by notes as was used above. For example, to send the request for help interactively from an IBM computer operating under VM, type:

TELL GRAND AT LSUCHE HELP

There are two limitations to sending a command interactively, however. The user must be using a direct BITNET link (rather than another net work such as ARPANET) and information cannot be added to files using interactive commands. For information retrieval, however, as well as initial signup and subscribing to a particu-

lar topic, the interactive method is easy to use and may provide a more rapid response. The general form of the interactive commands is:

TELL GRAND AT LSUCHE command

For all but the initial signup command (described below), the command should also be preceded by the words CONF CACHE to tell GRAND that the CACHE bulletin board is to be accessed.

GETTING STARTED: Signup and getting files.

Assuming that the network connection was tested and found to be working using the methods described above, the first step in actually using the bulletin board is to get it to recognize you by sending the command:

SIGNUP name

Your name should appear in this command in the form John Q. Smith, etc. This command should be sent in a mail note or as an interactive message as described above. GRAND will respond with a file called GRAND PROFILE which should be received and saved. Upon receipt of the file, you are ready to access the bulletin board.

To see the bulletin board subject areas, send the commands

CONF CACHE GET CACHE DIRECTRY

If you use an interactive message, these can be typed on one line; otherwise type them on separate lines within your note. The bulletin board will respond with a file that contains the main subject areas of the conference. The file has a number of lines that provide formatting for the CONFER interface program. For nonCONFER users, utilities are being developed that will discard these special lines. If you use the IBM/VM editor XEDIT, you can get the XEDIT macro file CACHE XEDIT from the bulletin board with the GET CACHE XEDIT command.

If you currently have neither CONFER nor an editor utility, browse the directory file and focus your attention on the lines that are not preceded by an exclamation mark. The bulletin board subjects are listed by name followed by the word "index." These represent the filename (subject name) and filetype (INDEX) of a particular file that is stored in the bulletin board. These files are all indexes to files that contain the actual bul-

letin board information. For example, to determine the specific files that make up the CAST (Computer and Systems Technology Division of AIChE) subject, send the commands: CONF CACHE and GET CAST INDEX. The file CAST INDEX that is returned to you will contain a listing of topics that are part of the subject area. Each of these topics represent individual files with their own filename and filetype. Any of these individual files can then be retrieved in the same manner as the indexes. For example, to retrieve the September newsletter of the CAST Division (if it existed on the bulletin board in a file SEPT NEWSLTTR) send the commands, CONF CACHE and GET SEPT NEWSLTTR.

Note that only part of a topic (file) can be retrieved by using the following GET commands with the filename (fn) and filetype (ft).

GET fn ft <entry #> (GET fn ft 1-5) GET fn ft SINCE <date> <time> (GET fn ft SINCE JUN) GET fn ft BEFORE <date> <time> (GET fn ft SINCE 6/22 11:00)

The entry number can be a single entry (c.g., 2) or a range (2-5) and the date and time can be given in a number of different formats.

OTHER COMMANDS

In addition to the ability to retrieve information with the "GET filename filetype" command, three other commands will be useful to most users. These are:

ADD (information)
JOIN ("subscribe" to a topic)
LEAVE (cancel a "subscription")

To add information to a topic (i.e., an individual file in a subject area) send the commands:

CONF CACHE
ADD filename filetype
start information to be added

· · · · · ·

end information to be added

The filename and filetype is the particular topic to which information is to be added. These can be determined from the list contained in the appropriate index (e.g., CAST INDEX will contain the list of all topics in the CAST subject). Note that the bulletin board will not allow you to add a new topic or to add information to an index. These requests will be routed to the bulletin board

operator at LSU.

The final two commands allow a user to establish or cancel a subscription to a topic. When a user subscribes to a topic, notification of all updates that are made to that topic are sent to that user. In this manner a response to a previous entry in a conference or a new program entry in a software library will be announced to all interested users.

Again, the filename and filetype of the particular topic in which the user is interested must be identified through the appropriate subject index. The user can then subscribe by sending the commands:

CONF CACHE
JOIN filename filetype

To drop a subscription and stop receiving update announcements, send the commands:

CONF CACHE LEAVE filename filetype

Note that it is also possible to subscribe to a particular subject area by joining the subject's index (e.g., CAST INDEX); then, any new topics in the subject area will be announced to you when an appropriate entry is made in the index.

WHAT NEXT?

The commands outlined in this article should help you to access and retrieve information on the LSU/CACHE Bulletin Board. In addition they provide you with the capability of contributing to the bulletin board. If you wish to contribute entries within a topic, please do so. The success of the bulletin board is entirely dependent on the willingness of the chemical engineering faculty to use the system and that, of course, is dependent on the quality and quantity of its offerings. If you have a more substantial contribution that you would like to make, i.e., one that merits an entire topic or even a new subject area, send the information or a message about the information to CMREIB at LSUCHE (BITNET address) or to:

Danny D. Reible Department of Chemical Engineering Louisiana State University Baton Rouge, LA 70803 (504) 388-1426

COMPUTER AIDED PROCESS OPERATIONS (FOCAPO)

edited by G. V. Reklaitis and H. D. Spriggs Published by Elsevier Science Publishers

This volume contains the proceedings of the First International Conference on Foundations of Computer Aided Process Operations (FOCAPO) held July 5-10, 1987 in Park City, Utah, USA. The Conference was sponsored jointly by the Computing and Systems Technology (CAST) Division of the American Institute of Chemical Engineers and the not-for-profit CACHE Corporation. The FOCAPO Conference, the first to deal specifically and exclusively with the problems of process or plant operations, had three objectives:

- 1) Define and discuss the problems of plant operations;
- 2) Report on the development and application of computing and computation tools and techniques for solving these problems; and
- 3) Bring together leading academic and industrial representatives to promote increased future interaction and cooperation in defining and solving operations problems.

Subjects covered in the Proceedings include (1) process data acquisition and interfaces, (2) process safety, (3) operations planing, (4) maintenance planning, (5) process simulation, (6) process optimization, (7) plant networks and databases, and (8) intelligent systems in process operations. The volume contains the manuscripts of all invited and contributed papers and summaries of the discussions which followed the papers.

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Process Safety

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Modelling and Simulation in Process Operation A Block Structured Approach to Dynamic Process Simulation Equation Based Process Simulation

Process Optimization

Mathematical Programming and the Planning, Scheduling and Control of Process Operations Retrofit Design of Processes

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Computer Aided Process Operations (FOCAPO) may be ordered from Elsevier Science Publishers, P.O. Box 211, 1000 AE Amsterdam, The Netherlands, or P.O. Box 1663, Grand Central Station, New York, NY 10163.

CHEMICAL PROCESS CONTROL—CPCIII

edited by M. Morari and T. J. McAvoy Published by Elsevier Science Publishers

This volume contains proceedings of the Third International Conference on Chemical Process Control, Asilomar, January 12-17, 1986.

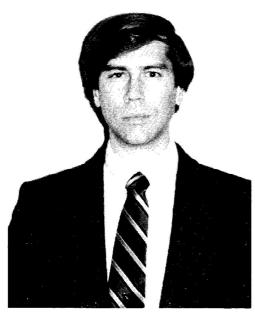
In these proceedings, conference participants from industry, government and universities discuss and critically review the current state of process control. The papers focus on advances that have taken place over the last five years, highlighting, in particular, developments in control system robustness, process operability, adaptive control, and mocel predictive control. New results on on-line identification and optimization, reactor control, and actual industrial applicatins of advanced control are also presented, and the potential impact of artificial intelligence and expert systems is assessed.

Specific topics covered are:

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CACHE WELCOMES NEW TRUSTEES AND OFFICERS

Jim Davis was elected to the CACHE board of trustees in November, 1987. Currently with the Department of Chemical Engineering at The Ohio State University, his interests lie in computer applications both in research and teaching.



Jim's research work centers artificial intelligence in process operations and design, and he is affiliated with the Laboratory for Artificial Intelligence Research at Ohio State. Teaching responsibilities include process control and process design. Before entering an academic profession, Jim spent three years with Amoco Chemicals working in plant operations, and prior to his appointment at Ohio State, he was a lecturer for two years in the Department of Mechanical Engineering at the University of Wisconsin-Madison. He received his B.Ch.E. degree from the University of Illinois and his M.S. and Ph.D. degrees from Northwestern University. With respect to CACHE activities, Jim is presently involved with the Task Force on Artificial Intelligence in Process Engineering.

Besides his interests and duties in chemical engineering, Jim is an avid pilot, runner, and scuba diver.

Professor Arkun is a native of Istanbul, Turkey. He received his B.S.ChE. from the University of Bosphorous, Turkey, in 1974 and the M.S.ChE. and Ph.D. degrees from the University of Minnesota in 1976 and 1979, respectively. From 1979 to 1985 he was on the faculty at Rensselear Polytechnic Institute. He joined Georgia Tech in July 1985, where he is currently an Associate Professor of Chemical Engineering.

Dr. Arkun is a member of AIChE, IEEE, and an associate editor of Automatica, the Journal of the International Federation of Control. He is the Chairman of the Systems and Control Area 10B of AIChE, and the recipient of the 1986 Donald P. Eckman Award given by the American Automatic Control Council.

Dr. Arkun has over 40 publications in the areas of process control and design. Dr. Arkun's research topics in process control include: modelling needs for control, design of robust controllers considering uncertainty, synthesis of control structures for chemical plants and design of



decentralized controllers, nonlinear and predictive control, application of modern methods to control of distillation columns, large scale integrated plants, batch processes and reactor systems. In the area of computer assisted control engineering, some of his recent studies concern: development of computer-aided multivariable control system analysis and design software, and expert systems for on-line optimization and constraint control.



Jeffrey J. Siirola is a Research Associate at the Advanced Process Technology Research Laboratory in the Eastman Chemicals Division of Eastman Kodak Company in Kingsport, Tennessee. He was elected Vice President of CACHE in March. Dr. Siirola has been an industrial trustee of CACHE since 1983 and chairs the Process Engineering Task Force. He has also been very involved in AIChE, ACS and AAAI (American Association for Artificial Intelligence).

After receiving his B.S.Ch.E. from the University of Utah, Dr. Siirola pursued a Ph.D. in chemical engineering from the University of Wisconsin—Madison. His main interests lie in chemical process computer-aided process design and non-numeric computer programming. He has written many articles and coauthored the book *Process Synthesis* in 1973.

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CACHE Process Design Case Study Vol. 2 DESIGN OF AN AMMONIA SYNTHESIS PLANT

Preliminary Design and Economic Analysis

Summary: The objective of the case study is the design of an ammonia synthesis plant that is to be built in 1990, and that uses hydrogen and nitrogen feedstocks from a coal gasification plant. All stages of the design procedure starting from preliminary calculations down to the detailed flowsheet calculations are described. Emphasis is placed on the following steps: screening of key flowsheet decisions (pressure of synthesis loop, ammonia recovery, synthesis of gas recycle, hydrogen recovery from purge stream), selection of reactor configuration, cost minimization, and synthesis of heat exchanger network.

The proposed design incorporates a medium-pressure synthesis loop with water absorption/distillation for

ammonia recovery, and with membrane separation for hydrogen recovery. The process was designed with the simulator PROCESS from Simulation Sciences, and the ammonia reactor was designed with the special purpose package QBED. A listing of this program is included in the case study. Depending on the required detail and the availability of process simulation software, the case study is suitable as a one-term assignment for a single student or a group of students. The preliminary calculations of the case study were performed by a group of three students, while the final design report is based on the work of a group of five students.

The problem statement was supplied by Philip A. Ruziska from Exxon Chemicals, and the case study was prepared under the supervision of Ignacio E. Grossmann from Carnegie-Mellon University.

CACHE PROCESS DESIGN CASE STUDY VOLUME 2

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CACHE Process Design Case Study Vol. 3 DESIGN OF AN ETHANOL DEHYDROGENATION PLANT

Preliminary Design and Economic Analysis

Summary: The objective of this case study is the preliminary design of an acetaldehyde synthesis process by ethanol dehydrogenation. The project covered all stages of the design procedure starting from consideration of qualitative aspects of the flowsheet and preliminary calculations to detailed process simulations and final economic evaluations. In this study emphasis is placed on synthesizing a workable flowsheet and justifying its configuration, simulating and evaluating the design using a commercial process simulator, and deriving a heat recovery network for the final process.

The main reaction in this process is the endothermic dehydrogenation of ethanol to acetaldehyde. However, under the specified reactor conditions, a number of byproducts are produced and their presence determines a number of interesting alternatives for separation. Once these alternatives have been screened and a workable flowsheet has been synthesized, the study centers on the simulation of this flowsheet using PROCESS from Simsci, Inc. Here, some of the features, advantages and limitations of this simulator are presented. Finally, the study concludes with a complementary presentation of this process simulated with the CACHE version of FLOWTRAN. While the aim of this study is not to provide a detailed comparison between PROCESS and FLOWTRAN, a useful description of the relative merits of both simulators can be readily observed.

This project is suitable for a one-term project by a five or six person team of senior design students. The results of two such teams are given in this study.

This problem was posed by the Union Carbide Corporation and the case study was prepared under the supervision of L.T. Biegler of Carnegie-Mellon University and R.R. Hughes of the University of Wisconsin.

CACHE PROCESS DESIGN CASE STUDY VOLUME 3

"Design of an Ethanol Dehydrogenation Plant"

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WHAT IS CACHE?

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

CREATION OF THE CACHE CORPORATION

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

CACHE ACTIVITIES

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

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

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