CACHE NEWS

News About Computers In Chemical Engineering Education.

No. 16

April 1983

WHAT IS CACHE?

CACHE is a non-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 1960's, 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, 14 chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. Initially, the CACHE Committee was 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 on-going projects. Information on CACHE activities is regularly disseminated through CACHE News, which is published twice each year. Individual inquiries should be addressed to:

CACHE Corporation
Room 3062 MEB
Salt Lake City, Utah 84112
(801) 581-6916

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CACHE NEWS

The CACHE News is published two times a year to report 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 above address. This issue was edited by J. D. Seader with contributions from a number of CACHE members and representatives.

TABLE OF CONTENTS

NEW CACHE TRUSTEE

At the November 19-20, 1982, meeting of CACHE, Dr. John H. Seinfeld was elected as an academic trustee. Dr. Seinfeld is currently the Louis E. Nohl Professor of Chemical Engineering and Executive Officer for Chemical Engineering at the California Institute of Technology. He received his Ph.D. at Princeton University, following which he joined the faculty at Cal Tech. Among a number of honors and awards, he received the Allan P. Colburn Award of the AIChE in 1976 and was the 32nd Institute Lecturer of the AIChE in 1980. He is a member of the National Academy of Engineering and has authored 3 books and 160 technical articles. His areas of research include mathematical modeling of air pollution, environmental reaction engineering, and applied mathematics.

FOCAPD-83 CONFERENCE

More than 125 chemical engineers are expected to attend the second conference on Fundamentals of Computer-Aided Process Design (FOCAPD-83) to be held June 19-24, 1983, at the Snowmass resort near Aspen, Colorado. The conference is being sponsored by the CAST (Computing and Systems Technology) Division of AIChE, the National Science Foundation, and CACHE, with the latter being responsible for all arrangements. Professor Arthur W. Westerberg of Carnegie-Mellon University and Dr. Henry H. Chien of Monsanto Company are conference chairman and co-chairman, respectively.

Nine successive sessions will be held during the five-day period. The focus of the meeting will be the presentation of both industrial and academic viewpoints on computer-aided design, with about 90 minutes of each session devoted to discussion of issues raised by the speakers. The program for the meeting is as follows:

Keynote Address:
"Can 'Expert' Systems Solve Technological Problems?"
Speaker: Peter D. Hart
Fairchild Advanced Research & Development

Session I: "Overview and Outlook"
Chairman: Jerry L. Robertson
EXXON Research & Engineering

Speaker: Roger Sargent
Imperial College, London
"Challenges and Constraints in Computer Science and Technology"

Speaker: Stanley I. Proctor
Monsanto Company
"Challenges and Constraints in Computer Implementation and Applications"

Session II: "Progress in Data Base Development"
Chairman: Theodore L. Leininger
DuPont Company

Speaker: Peter Winter
CAD Center, Cambridge, England
"Data Base Frontier in Process Design"

Speaker: R. Peter Dube
Boeing Computer Services
"Data Base Technology Applied to Engineering Data"

Speakers: Raymond A. Lorie and
Wilfred Plouffe
IBM Corporation
"Relational Data Bases for Engineering Data"

Session III: "Computational Algorithms"
Chairman: Gary E. Blau
Dow Chemical

Speaker: Gordon Bradley
Naval Post Graduate School
"Mixed Integer Programming"

Speaker: Warren D. Seider
University of Pennsylvania
"Physical Insights to Aid in Model and Algorithm Formulation"

Session IV: "Physical Properties for Design"
Chairman: Joseph Boston
ASPENTech

Speaker: John P. O'Connell
University of Florida
"The Structure of Thermodynamics in Process Calculations"

Speaker: Edward A. Grens
University of California, Berkeley
"Efficient Use of Thermodynamic Models in Process Calculations"

Session V: "Nonsequential Modular Flowsheeting"
Chairman: Rodolphe L. Motard
Washington University

Speaker: John D. Perkins
Imperial College, London
"Equation-Oriented Flowsheeting"

Speaker: Lorenz T. Biegler
Carnegie-Mellon University
"Simultaneous Modular Simulation and Optimization"

Session VI: "Design and Scheduling of Batch Chemical Plants"
Chairman: Richard S. H. Mah
Northwestern University

Speaker: G. V. Reklaitis
Purdue University
"Intermediate Storage in Non-Continuous Processes"

Speaker: Harold N. Gabow
University of Colorado
"On the Design and Analysis of Efficient Algorithms for Deterministic Scheduling"

Session VII: "Complex Single Unit Design"
Chairman: Bruce A. Finlayson
University of Washington

Speaker: Warren E. Stewart
University of Wisconsin
"Collocation Methods in Distillation"

Speaker: H. H. Klein
JAYCOR Scientific Research & Development
"Modeling Fluidized-Bed Chemical Reactors"

Session VIII: Contributed Papers
Chairman: Cameron M. Crowe
McMaster University

Title of Paper
Author(s), Affiliation

"Scheduling of Multipurpose Batch Plants with Product Precedence Constraints" by
I. Suhami, EXXON, and
R. S. H. Mah, Northwestern University

"The Prediction of Properties and Its Influence in the Design and Modeling of Superfractionators" by
M. R. Hernandez, R. Gani (Speaker),
J. Romagnoli, and E. A. Brignole,
Universidad Nacional del Sur, Argentina

"Reduced Cost Solutions to Multistage, Multicomponent Separations Problems by a Hybrid Fixed-Point Algorithm" by
K. R. Westman and A. Lucia (Speaker),
Clarkson College of Technology, and
S. Macchietto, Imperial College

"Solution of Systems of Complex Interlinked Distillation Columns by Differential Homotopy-Continuation Methods" by
T. L. Wayburn and J. D. Seader (Speaker),
University of Utah

Strategies for Simultaneous Modular Flowsheeting and Optimization" by
M. A. Stadtherr (Speaker) and H.-S. Chen,
University of Illinois - Urbana

"Recent Developments in Solution Techniques for Systems of Nonlinear Equations" by
M. Shacham, Ben-Gurion University of the Negev

Session IX: "Operability in Design"
Chairman: George Stephanopoulos,
National Technical University, Athens

Speakers: Ignacio Grossmann,
Carnegie-Mellon University, and
Manfred Morari,
University of Wisconsin

"A Dialogue on Resiliency, Flexibility, and Operability - Process Design Objectives for a Changing World"

The proceedings of the conference will be published by CACHE following the meeting. Each attendee will receive a copy of the proceedings. Those unable to attend the conference may order a copy of the proceedings from CACHE. Additional information on the conference can be obtained by calling Vickie Jones at (801) 581-6915 in Salt Lake City, Utah.

The two-volume set (1178 pages total) of the proceedings of the first FOCAPD Conference held in 1980 is available for $40 to AIChE members from AIChE.

FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

As part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program will be made available on magnetic tape to departments of chemical engineering to install on their own in-house computers. Thus, departments will be able to run FLOWTRAN on their own computers at no charge other than that of their own computer center. CACHE will have the responsibility of preparing the load modules for a wide variety of main-frame-type digital computers and for distributing the modules on magnetic tape to those departments that order them. Instructional books on FLOWTRAN are already available thrugh CACHE. An order blank is given near the end of this newsletter.

CACHE has initiated this new FLOWTRAN project at the University of Utah, the University of Michigan, the University of Akron, Rice University, and Worcester Polytechnic Institute for UNIVAC, Amdahl, IBM, VAX, and DEC 10 and 20 computers, respectively. As a former, current, or future user of FLOWTRAN, you may be interested in ordering a load module, subject to a moderate cost and to approval by Monsanto Company. If you have not already done so, contact:

CACHE
MEB 3062
Salt Lake City, Utah 84112
(801) 581-6916

PROGRAMS FOR HAND-HELD PROGRAMMABLE CALCULATORS

Professor F. William Kroesser of West Virginia College of Graduate Studies has just completed a CACHE booklet entitled **"Hand-Held Programmable Calculators: A Review of Available Programs for Chemical Engineering Education."** In this 26-page booklet, approximately 100 programs are listed under the following subjects:

THERMODYNAMICS
- Thermodynamic Properties
- Equations of State
- Equilibria

TRANSPORT PHENOMENA
- Viscosity
- Bernoulli Equation
- Pipe Flow
- Open Channel and Wier Flow
- Conduction
- Convection
- Radiation
- Diffusivity

UNIT OPERATIONS
- Distillation
- Absorption
- Humidification and Cooling

PROCESS DESIGN AND CONTROL
- Control Valve Size
- Fluidized Beds
- Compressors

Given for each program listed are 1) a description, including restrictions, 2) a literature reference to the program listing, and 3) a summary of input and

HP67/97 Users' Libraries, the TI58/59 Program Exchange Club and specialty booklets, and articles in Chemical Engineering, Chemical Engineering Progress, Hydrocarbon Processing, and the Oil and Gas Journal.

An order blank for Professor Kroesser's booklet is included at the end of this issue of CACHE News.

TASK FORCE FOR THE DEVELOPMENT OF PROCESS DESIGN CASE STUDIES

by Manfred Morari

The CACHE Task Force on Process Design Case Studies, under the direction of Professor Manfred Morari, has completed the preparation of two problem statements that have been submitted to those expressing interest. The first problem, entitled **"Solvent Recovery System,"** was prepared by Dr. J. J. Siirola of the Tennessee Eastman Co. It involves the preparation of alternative flowsheets to separate a mixture of three organic compounds and water, which forms two liquid phases over most of the composition range. This problem requires consideration of energy and heat integration and tests techniques for the synthesis of separation trains.

The second problem, entitled **"Ammonia Synthesis,"** was provided by Professor I. Grossmann of Carnegie-Mellon University in cooperation with EXXON Research and Engineering Co. This is a rather large problem suited for groups of students and is solved best with computer-aided simulation programs as an aid in synthesis and optimization.

These two problems have been prepared in line with the following guidelines developed by the Task Force:

General Philosophy:

The CACHE Case Studies are to be tutorial with both the instructor and the student in mind. Thus the stated problems and published reports will generally be distinctly different from AIChE contest problems, for example, and from reports prepared for an industrial setting. The problems will usually be loosely defined; a flowsheet will often not be specified. The goal is not necessarily to present one "optimal" solution, but possible several alternatives with different attractive features. One section of the report should show in detail the steps how, starting from the problem statement, alternative solutions were generated and discarded based on prelminary short-cut calculations and qualitative considerations, and how the number of alternatives is decreased by the designer as he progresses toward a final solution. It should demonstrate how simplifying assumptions can unclutter detail and lead to reasonable but not necessarily, in the mathematical sense, optimal solutions.

Scope:

The eventual goal is to have a library of case studies ranging from small projects that can be completed by one student in a matter of, say, one month to large ones that will require the coordinated effort of a group of maybe four students extending over a whole semester. In the current initial phase of the Task Force, projects of any scope are welcome. It is important to emphasize that a list with detailed equipment specifications is not necessarily the final goal, but a well-thought-out preliminary analysis presented in a tutorial manner can be equally valuable.

Design Techniques

It is desired to demonstrate a variety of different design techniques through the CACHE Case Studies. In the present initial period of existence of the Task Force, it is up to the preference and expertise of the Task Force member which technique he wishes to use. Eventually, the Task Force would like to see among the applied principles and methods:

Process Synthesis, in particular, synthesis of separation trains and energy management systems (heat exchanger networks, heat pumps, and heat engines).

Flowsheeting and the application of steady-state simulators; for example FLOWTRAN

Optimization

Design of complex unit operations, e.g., reactors and nonstandard distillation columns

Physical Property Estimation

For further information, contact:

Professor Manfred Morari
Dept of Chemical Engineering
University of Wisconsin
1415 Johnson Drive
Madison, WI 53706
(608) 262-1092

THIRD AND FOURTH CACHE SHORT COURSES ON MICROCOMPUTER INTERFACING/PROGRAMMING

CACHE would like to thank Professor David Graves and the Department of Chemical Engineering at the University of Pennsylvania for hosting the third CACHE short course on microcomputer interfacing/programming from October 21 through October 25, 1982. Half of the participants were chemical engineering graduate students, several of whom traveled substantial distances to attend the course. Attendees included:

Dr. Prasad Dhurjati, Univ of Delaware
Dr. Jack Famularo, Manhattan College
Dr. E. K. Grunwald, Energy Analysis, Inc.
Dr. J. Christopher Ludlow, West Virginia Univ
Dr. Janice A. Phillips, Lehigh Univ
Dr. Paul Schubert, Polytech Inst of New York

Graduate Students
Mark Burns, Univ of Pennsylvania
Chun-Sheng Ko, Univ of Pennsylvania
Tore Lindstrom, Univ of Southern California
Joseph Mclaughlin, Rice Univ
Rick Nelson, Rice Univ
Kostantinos Tsakalis, Univ of Southern California
Diego Valenzuela, Univ of Pennsylvania

A one-day introduction to basic concepts of digital electronics was followed by a four-day introduction to microcomputer programming (machine code, assembly language) and microcomputer interfacing. A new Z80-based microcomputer trainer, the FOX (E & L Instruments, Inc.), along with associated texts and laboratory workbooks, permitted a streamlining of the lectures and laboratory interfacing experiments. Participants were allowed to take the equipment to their homes or motel rooms for additional work during the evening. The average cost of the course, not including travel or lodging expenses, was approximately $123, which included the purchase of the FOX Modules 1, 2A, and 2B and two additional textbooks.

CACHEcourse No. 4, a repeat of CACHEcourse No. 3, is being considered for the summer (August 1983), the fall (October 1983), or the winter (January or February 1984). Both chemical engineering faculty and graduate students are encouraged to attend. We still need to identify a host institution. If you are interested in being a host institution or in having graduate students or faculty from your department attend the short course, please send your name along with your first, second, and third choices for short course date to

Dr. Peter R. Rony
Department of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, Virginia 24061
(703) 961-6370)].

One possibility for a host institution (July 25-29, 1983) is Virginia Polytechnic Institute & State University. Inexpensive camping facilities would be available at Claytor Lake State Park (35 miles away) for those participants who would like to cut costs to the bone. Since the instructor would not need to pay travel or lodging expenses to a host site, short course costs would be limited essentially to the cost of books ($30 to $40), microcomputer rental ($25), lodging, and travel. Virginia, a very scenic state that is popular with tourists, has numerous attractions such as Monticello, the Blue Ridge Parkway, Civil War sites, caverns, and, of course, scenic downtown Blacksburg.

MICROCOMPUTER TASK FORCE: THE NOVEMBER 14, 1982, QUESTIONNAIRE

About 150 chemical engineering departments received a questionnaire that probed current work, by chemical engineering faculty, with microcomputers or personal computers in laboratory applications such as real-time control, data logging, system timing, etc.; the availability of information on such work, including reports, articles, and theses, suggested activities for the CACHE Microcomputer Task Force and potential interest in "CACHE consultants." Forty-three departments have responded to date.

The evaluation of data and the writing of a report are being delayed pending the receipt of additional questionnaire responses. Many of the replies received to date are so interesting that it makes sense to get more complete data. Any department of chemical engineering in the United States, Canada, and Mexico would render a substantial service to chemical engineering education by sending its response, thus permitting CACHE to develop a complete snapshot-in-time of microcomputer resources in chemical engineering. Only two people will see the raw data (which will be regarded as confidential) and write the report. Our objective will be to present the overall picture and not to focus on specific departmental situations, good or bad.

For additional copies of the questionnaire, please contact:

Dr. Peter R. Rony
Dept of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, VA 24061

SPECIAL WASHINGTON, D.C., SESSION: "INTRODUCING/UPDATING REAL-TIME COMPUTING IN THE UNDERGRADUATE LABORATORY"

The CAST Division of AIChE and the CACHE Corporation are initiating a new program that has as its primary objective the updating of chemical engineering departments on important aspects of the rapid changes in the educational use of computers. As the first joint activity of these two organizations, a special, non-regularly scheduled technical session is being planned for the Washington, D.C., AIChE meeting during October/November, 1983. Additional sessions will be planned for future AIChE meetings.

The title of the initial CACHE/CAST session is "Introducing/Updating Real-Time Computing in the Undergraduate Laboratory." It will be held at the Washington, D.C. Hilton Hotel on Sunday, October 31, 1983, from 8 to 10 p.m. (after the AIChE cocktail hour), which hopefully will be a convenient time for the 50-75 people who are expected to participate.

CONTRIBUTIONS TO THIS SESSION ARE SOLICITED FROM CHEMICAL ENGINEERING FACULTY. Time will be available for three or four presentations. Those who are potential contributors may be interested in a CACHE report (based upon a November 14, 1982, CACHE Microcomputer Task Force Questionnaire, which probed faculty opinions on a variety of aspects associated with real-time computing in ChE departments) that will be published during the spring. This report should give you perspective on the hardware that currently exists in chemical engineering departments, the availability of reports and expertise associated with specific computer systems, the time required to develop laboratory experiments, and the perceived needs for assistance and information.

If you would like to give one of the presentations at the CACHE/CAST Washington, D.C., special session, please check the appropriate box on the form at the end of the newsletter and submit an abstract, by the **July 31, 1983**, deadline, to the session chairman listed below. Departments who would like to reserve a place at the session for their representatives are encouraged to check the appropriate box and return the tear sheet to the session chairman.

Professor Peter R. Rony, CACHE/CAST Session Chairman
Department of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, VA 24061

Professor Michael B. Cutlip, CACHE/CAST Session
Vice Chairman
Department of Chemical Engineering
University of Connecticut
Storrs, CT 06268

CAST DIVISION SESSIONS FOR FUTURE AIChE MEETINGS

The CAST Division of AIChE has planned the following technical sessions for the October-November, 1983, and May, 1984, meetings at Washington, D.C., and Anaheim, respectively.

Washington, DC Diamond Jubilee Meeting
(October 30 to November 4, 1983)

Six sessions are planned:

1. **Computers in Process Analysis and Synthesis**
   M. Morari, Wisconsin - Chairman
   C. Brosilow, Case-Western - Vice Chairman
2. **Applied Mathematics in Chemical Engineering**
   S. W. Churchill, Univ Pennsylvania - Chairman
   D. Ramkrishna, Purdue Univ - Vice Chairman

3,4. **Major New Directions in Process Control I & II**
   D. Seborg, Univ California, Santa Barbara - Chairman
   J. D. Wright, Xerox, Canada - Vice Chairman

5,6. **Computer-Aided Process Engineering**
   I. Preliminary Design
   II. Design Execution
   F. M. Rosen, Monsanto - Chairman
   B. Dickert, Union Carbide - Vice Chairman

The programs for the sessions are nearly complete and will be frozen April 15, 1983.

Anaheim Annual Meeting
(May 20 to 24, 1984)

The Anaheim meeting will feature Computers in Chemical Engineering as a theme. The CAST Division is sponsoring the following 11 sessions:

1. **Process Modeling with Computers**
   H. Britt, ASPENTech - Chairman
2. **Process Data Reconciliaton and Rectification**
   R. S. H. Mah, Northwestern - Chairman
3. **Human Factors in Computer Control**
   (Chairman unassigned)
4. **Software for Advanced Computer Control**
   (Chairman unassigned)
5. **Software for Control System Design**
   (Chairman unassigned)
6. **Progress Towards Process Engineering Workstations**
   F. M. Rosen, Monsanto - Chairman

The other five sessions will explore the role of micro or personal computers in chemical engineering. Vendor displays will be organized at the Exposition to parallel these sessions.

7. **State-of-the-Art Review**
   B. Finlayson, Univ of Washington - Chairman
   M. Tayyabkhan, Mobil R & D - Vice Chairman
8. **Microcomputers in the Laboratory**
   P. Rony, Virginia Poly Inst & State Univ - Chairman
9. **Microcomputers in Education**
   B. Carnahan, Univ of Michigan - Chairman
10. **Microcomputers in Professional Practice**
    N. Rawson, IBM - Chairman
11. **Pros/Cons of Microcomputers: Panel Discussion**
    M. Tayyabkhan, Mobil R & D - Chairman
    M. Sood, Mobil R & D - Co-Chairman

Authors with potential contributions for these sessions are invited to submit them to the session chairmen. For further information, contact:

Professor G. V. Reklaitis
School of Engineering
Purdue University
West Lafayette, IN 47907
(317) 494-4089

3RD INTERNATIONAL CONGRESS ON COMPUTERS AND CHEMICAL ENGINEERING PARIS, FRANCE

This annual computationally oriented meeting sponsored by the European Federation of Chemical Engineers is being held April 19-21, 1983. The program has been distributed, and bound preprint volumes will be printed in advance of the meeting. The preprints are available through the **Societe de Chimie Industrielle, 28, rue Saint Dominique, F-75007 Paris, FRANCE.**

The meeting features plenary lectures by Professor Takeichiro Takamatsu (Kyoto University, Japan), **"The Present Status and Future Aspects of Process Systems Engineering in Japan,"** and by Professor Warren D. Seider (University of Pennsylvania), **"Generalized and Specialized Algorithms in Chemical Process Analysis."**

A total of 175 papers will be presented on topics such as Flowsheeting, Simulation of Reactors and Separations Systems, Process Control Applications, and Numerical Problems. The final program includes the following seven papers from the United States:

1. A. I. Majeed and J. H. Erbar, **"Interactive Process Design on Microcomputers."**
2. D. M. Himmelblau, **"Instrument Fault Detection by Using Internal Redundancy."**
3. M. A. Stadtherr and H.-S. Chen, **"Numerical Techniques for Process Optimization by Quadratic Programming."**
4. L. T. Biegler, **"Improved Feasible Path Methods for Sequential Modular Optimization."**
5. A. I. Avidan and I. E. Grossmann, **"FLEXPACK - A Computer Package for Optimal Multiperiod Design."**
6. S. A. Shah, M. R. Okos, and G. V. Reklaitis, **"A Multiperiod Production Planning Model for Food Processing Plants."**
7. G. Joglekar, S. Clark, and G. V. Reklaitis, **"BOSS: A Process Simulator for Non-Continuous Operations."**

THIRD PACIFIC CHEMICAL ENGINEERING CONGRESS (PACHEC), Seoul, Korea

The final program of this meeting, sponsored by the Asian Pacific Confederation of Chemical Engineering and the InterAmerican Federation of Chemical Engineering, has been distributed. The meeting, to be held May 8-11, 1983, features plenary lectures by Dr. Klaus Mai of the Shell Development Company, **"Energy and Petrochemical Feedstocks - A View of the Future,"** Professor Tokuro Mizushina of Kyoto University, **"Special Research Projects in Japanese Universities,"** and Professor Gilbert Froment, Rijksuniversiteit (Belgium), **"Fixed-Bed Reactor Design."** Computationally oriented sessions include:

Process Modeling and Simulation
Process Dynamics and Control
Process Synthesis and Analysis
Computer Control and Graphics

The program includes some 35 contributions from the United States. Preprints will be published in four volumes and are available from the

PACHEC '83 Secretariat
c/o Dept of Chemical Engineering
Korean Advanced Institute of Science and Technology
Chongryang, P.O. Box 150
Seoul, KOREA

MEETING IN ENGLAND PLANNED ON THE USE OF COMPUTERS IN CHEMICAL ENGINEERING

The Institution of Chemical Engineers (Rugby, England) is proposing to organize a conference in Cambridge, England, at Robinson College on March 31 to April 13, 1985, on the use of computers in chemical engineering.

There will be no parallel sessions. No formal arrangements will be made for round-table discussions, but rooms will be set aside for informal gatherings.

Space will be provided for authors who are working on new areas/ideas that are not yet far enough advanced to present a full paper. This will take the form of a poster exhibition, and authors will be expected to make themselves available for discussion at prearranged times outside normal session times. This may overlap with the discussion arrangements. Space will be provided for an exhibition of software/hardware relevant to the themes of the Conference. This will be separate from the poster exhibition. Four or five papers of 30 minutes each (including discussion) will be accommodated per session, and each major session will have a Chairman-Rapporteur.

The conference proceedings will be published in the IChemE Symposium Series.

Appropriate visits, a social programme, and a ladies' programme will be arranged.

Provisional Timetable for Authors

Early 1984	Final Call for Papers
August, 1984	Deadline for abstracts
November, 1984	Draft of final paper
January, 1985	Final paper for printing

Comments or suggestions should be directed initially to:

F. A. Perris
Engineering & Scientific Systems Department
Air Products, Ltd
Hersham Place
Molesey Road
Walton-on-Thames
Surrey KT12 4RZ
ENGLAND

Proposed Themes for Conference

Operability Considerations at the Design Stage
- process dynamics
- hazard & operability studies
- fault trees
- availability & reliability
- measures of controllability
- flexibility/resilience

The Influence of New CAD Technology
- databases and databanks
- graphics
- integration of systems
- new hardware (e.g., micros and local area networks)

The Design of Flowsheets
- new flowsheeting technology
- batch & semi-batch processes
- multiphase systems
- synthesis of whole flowsheets
- costing and economic analysis

Aids for Plant Operation
- monitoring & analysis of plant performance
- fault detection/diagnosis
- reconciliation of measured plant data

The Management of Design
- useability of design systems
- issues of liability & responsibility
- uncertainty & risk

Notes:
The emphasis throughout the meeting will be on the presentation of new information on either technology or its application. Papers describing applications will be encouraged, especially if they contain information relating to the value of the study, estimated savings, etc., in reasonable detail. Papers that describe important new work in other areas of process engineering CAD will be considered for inclusion. In particular, the "poster session" will allow authors to present their latest ideas, which may not yet have reached a stage which justifies a full paper.

STATUS OF IAN DOIG'S PROCESS TROUBLESHOOTING EXERCISES

by
D. M. Himmelblau

One of the major activities of engineers is the identification and diagnosis of problems in plant operations. Typical problems arise that must be corrected immediately, or at least as soon as possible, with minimum cost. Very few areas in chemical engineering education treat such problems formally, and there is a definite need for improving the skills of students in solving such problem.

CACHE is preparing for distribution a program authored by Professor Ian D. Doig of the Department of Chemical Engineering at the University of New South Wales, Kensington, Australia. Professor Doig's program is the first to make substantial use of computer-student interaction in process fault diagnosis. Most attempts to engage in the improvement of skills in trouble-shooting have directed students to work on their own to determine the cause of the fault(s) in the process or work via groups, but the students obtain information from the instructor by asking questions about past experiences, the results of their calculatons, the results of experiments, etc. Also, usually the troubleshooting cases that are examined refer to single pieces of equipment or small collections of equipment. Often, emphasis is placed on developing a suitable strategy for solving the problem; and little effort goes into a realistic solution of the problem. What Professor Doig has accomplished is to set up a large data base of information that represents a flowsheet for a chemical plant. Data are made available on demand for measurements at a large number of locations in the plant for streams such as cooling water, steam, chilled water, and other utilities. In addition, measurements can be solicited as requested by the user on all the details of valves, pumps, blowers, and so forth, as well as physical data for all components of all streams.

Upon logging onto the computer, the student is presented with a corresponding set of current routine measurements, which differ significantly in some ways from the normally expected values. Consequently, a fault exists. The student calls for additional samplings and measurements until his hypothesis concerning the causes of the fault have been accepted or rejected. Over 100 possible faults exist in the system; and the constructor, by introducing code numbers, can select one or more of these.

For each ad-hoc sampling and measurement ordered by the student, he or she is charged an imaginary expense. The goal is to locate and identify the fault with a minimum cost.

Other features of the system that provide realistic representation of a plant include a randomly generated Gaussian distributed error that is contained in all the measured values reported. Also, a student can be asked to resolve two simultaneous malfunctions usually chosen to be noninteractive.

An instructor can use the computer program to develop student trouble-shooting skills, including: 1) realization that something is in error, 2) definition of the problem, 3) collection of data, 4) reaching conclusions about the data, 5) re-evaluation of the problem, 6) cycling of the analysis until the final diagnosis is complete.

It is expected that Doig's program, which is now being tested, will be available for distribution by CACHE in Spring, 1983. Any faculty member who would like to evaluate the program prior to general distribution should contact:

Professor D. M. Himmelblau
Dept of Chemical Engineering
The University of Texas
Austin, TX 78712
(512) 471-7445

ADDITIONAL ChE MATERIALS ON PLATO

by Michael B. Cutlip and
Stanley I. Sandler

CACHE News No. 15, September, 1982, listed on page 13 the chemical engineering lessons that are now available on the worldwide PLATO educational computer system of the Control Data Corporation. These lessons currently require a CDC PLATO terminal with a telephone connection to a central computer running the PLATO system. Additional work in the creation of new materials is continuing at several universities, and the following discussion is limited to lessons that are soon to be released by CDC. Current availability (before official release by CDC) can be determined by contacting the lesson authors.

NUMERICAL ANALYSIS - Two additional lessons have been added to the three lessons described in the last CACHE newsletter. The authors of this PLATO Numerical Computation Package are chemical engineering Professors Mordechai Shacham of Ben Gurion University of the Negev in Israel and Michael Cutlip of the University of Connecticut.

Multiple Linear and Nonlinear Regression Program - This lesson allows the user to input up to 20 experimental data points of the dependent variable y versus up to 4 independent variables X1,...., X4. Mathematical models containing up to 5 linear and up to 2 nonlinear parameters can be fitted to the original or transformed experimental data. Visual and numerical feedback regarding the goodness of fit are provided. Both the data and the mathematical model can be conveniently modified or updated.

Library Entry to the Computational Package - This utility lesson allows the serious user of the PLATO Numerical Computation Package to create a personal problem library to be used with all the following lessons:

1. Simultaneous Ordinary Differential Equation Simulator
2. Simultaneous Linear and Nonlinear Algebraic Equation Solver
3. Polynomial, Linear, and Nonlinear Curve Fitting Program
4. Multiple Linear and Nonlinear Regression Program.

The user can store problems and data in the library for future use. Convenient updating, modifying, and solution of modified problems are therefore available.

The collection of five lessons in numerical analysis has been developed to provide interactive problem-solving capabilities to students for use with coursework or projects. The PLATO terminal is very user friendly and requires no language. Students can learn to operate the terminal in approximately 1/2 hour of computer-based instruction. Each lesson of the PLATO Numerical Computation Package has a HELP section from which students can learn to use the lesson and obtain details on the underlying numerical methods. The lessons are highly interactive and allow the user to solve many realistic problems efficiently. Over 250 students have enjoyed testing these lessons.

THERMODYNAMICS - A package of 14 chemical engineering thermodynamics lessons prepared by Professor Stanley I. Sandler of the University of Delaware will be released by CDC in the near future. These lessons are meant to provide enrichment and tutorial material for thermodynamics courses. Below is a brief description of the lessons in this package.

EXPAN A complicated problem involving mass, energy, and entropy balances to solve an ideal gas expansion problem.

DESUPER A problem using mass and energy balances and the steam tables (a portion of which are provided) to solve a steam-flow problem.

TURB A problem using mass, energy, and entropy balances and the Mollier diagram (which is provided) to solve for the work obtained from a steam turbine operating in several different modes.

REPRESS Uses the mass and energy balances and the ideal gas law to solve several related problems on the compression of an ideal gas.

REFRIG The analysis of a Rankine refrigeration cycle using the mass, energy, and entropy balances and a displayed pressure-enthalpy diagram for a chlorinated hydrocarbon.

TANK 1 An introductory lesson on modeling fluid flow from a tank.

STATES 1,2 and 3 A series of lessons on the corresponding states principle and its application to chemical engineering problems.

MB3 A problem in stoichiometry involving an ideal gas-phase chemical reaction.

REACT 1 A lesson dealing with chemical equilbrium in an ideal gas-phase reaction system.

REACT 2 A continuation of the previous lesson complicated by the formation of a solid phase.

REACTU 1 A utility program, with attached data base for standard state heats and free energies of formation and heat capacities, which allows the student to quickly calculate and plot the equilibrium constant and heat of reaction as a function of temperature.

BINMIX A lesson which first provides instruction on the use of the Othmer still for obtaining vapor-liquid equilibrium data and then asks the student to determine which activity coefficient model best fits these data.

CHEMI PROJECT UPDATE

The second phase of the CHEMI project was funded in 1979 by a National Science Foundation grant to the CACHE Corporation with the objective of making the chemical engineering instructional modules developed during the first phase of the project available on-line. A major activity of the project, the design of the information system, was completed in 1982.

Most of the first version of the database retrieval system has been coded. The system includes facilities for: 1) use of an on-line glossary, 2) automatic index search for all modules containing a specific keyword, 3) convenient interactive presentation of all modules and abstracts, 4) printing of modules and abstracts, and 5) easy and immediate access to all applicable HELP files. It also includes rudimentary (but easily expandable) features for the storage of various system and user statistics and features to allow users to keep their own permanent records. Workspaces can easily be added. Still to be written is the Pathway search and determination facility that will assist the user in choosing the proper set of modules, in the correct order, necessary to reach a particular educational goal.

The system has been written in the "C" programming language and is running under the UNIX operating system on a DEC PDP-11/23 computer. The choice of C as a language makes the source code highly modular, so it can be easily expanded and tailored to fit specific needs. It also makes the system quite portable; C is a young language whose conventions have been standardized. UNIX is an extremely flexible operating system that has rapidly gained popularity among computer users in science and engineering.

The system allows on-line access to the modules through key-word search, sequence selection (the LINK program), abstracts, and an index. A module, part of a module, or any screen of information can be printed off-line if a printer is available. Pre-tests, mastery tests, homework, computer programs, and complex figures will be available only in a print supplement because the time and cost involved in coding interactive testing is prohibitive and because the standard ASCII terminal cannot display complex graphics. Coding of the CHEMI information system is in the programming language C.

We are presently working on entering data from the modules into the PDP-11/23 computer owned by the CACHE Corporation and the PDP-11/70 computer, which

is available through the Computation Center at the University of Texas, Austin. On both systems we are using the UNIX operating system, Version 7. We also store files on the CDC 170/750 computer at the Computation Center.

Retrieval of CHEMI will be on standard ASCII terminals such as ACTV's and ADM3's. Because of certain limitations in the graphics display on such terminals, we have developed guidelines for equation formatting that set standards for Greek letters, subscripts and superscripts, and certain mathematical symbols. Students in chemical engineering classes at the University of Texas, Austin, were asked to rank various equation formats as to preference. The results of this poll are the basis for the guidelines used in formatting the equations in the CHEMI modules. Transposing the equations from the original version to one that can be entered into the computer using a standard terminal is a task requiring patience and attention to detail.

Examples of original equations and figures and their computer counterparts can be seen in the following:

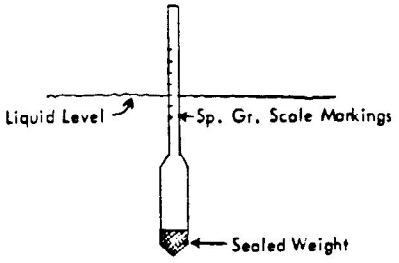
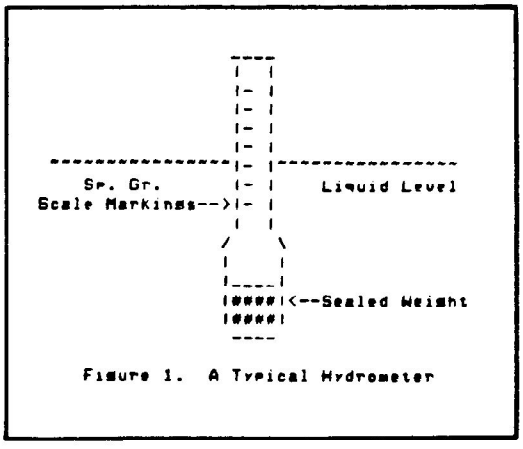


Figure 1. A Typical Hydrometer.

(a) Original Drawing



(b) On-Line Drawing (Module MEB 2)

FIGURE 2. Example of a Two-Dimensional Drawing

For a single stream, if we leave out the change in internal energy and divide both sides of Eq.(3) by the mass, m, being conveyed, we obtain the well known Bernoulli equation:

$$\Delta\left[\frac{P}{\rho}\right] + g\,\Delta Z + \frac{1}{2}\,\Delta u^2 = 0 \qquad (4)$$

where ρ is the density and $\Delta Z = Z_{exit} - Z_{entrance}$ etc. Eq. (4) is frequently referred to as a mechanical energy balance.

(a) Original Format (Module MEB 30)

For a single stream, if we leave out the change in internal energy and divide both sides of equation (3) by the mass, m, being conveyed, we obtain the well known Bernoulli equation:

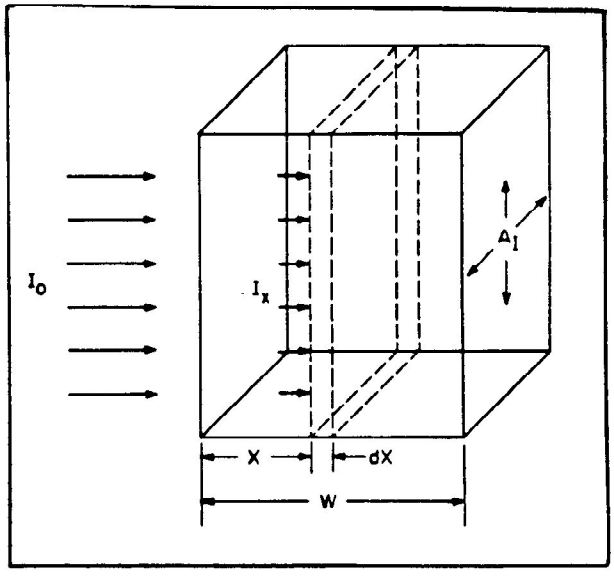
$$\text{DELTA}\left(\frac{P}{RHO}\right) + (g)[\text{DELTA}(Z)] + 1/2\ \text{DELTA}(u^2) = 0 \qquad (4)$$

where RHO is the density and DELTA(Z) = (Z_{exit} - $Z_{entrance}$) etc.

Eq. (4) is frequently referred to as a mechanical energy balance.

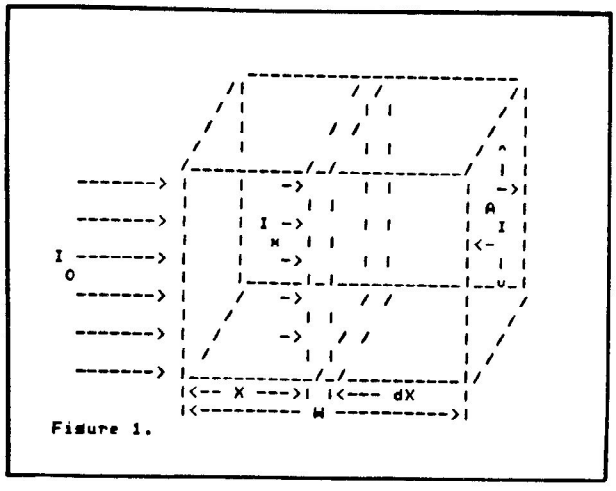
(b) On-Line Formatting (Module MEB 30)

FIGURE 1. Example of an Equation



(a) Original Drawing

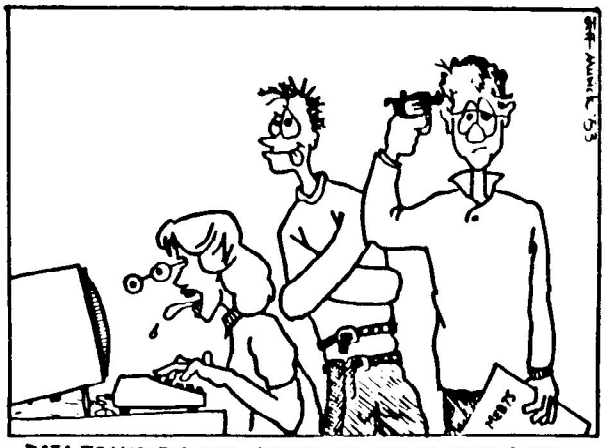
Physical Model for Determining the Average Algal Growth Rate (Module KIN 30)



(b) On-Line Drawing

Physical Model for Determining the Average Algal Growth Rate (Module KIN 30)

FIGURE 3. Example of a Three-Dimensional Drawing



MICROCACHE PROJECT REPORT

by Brice Carnahan

The first phase of the MicroCACHE project is now essentially complete. Although we are still making minor changes as a result of testing experience with students, the supervisory system for operation of the CAI (Computer-Aided Instruction) system has been completely coded and (we believe) thoroughly debugged for operation on an Apple II+ microcomputer (equipped with 64K of random-access main memory, two disk drives, a Microsoft Z-80 Softcard, and a monochrome monitor).

The thirteen prototype educational modules (lessons) listed below have been written and debugged:

1. McCabe-Thiele distillation
2. Ponchon-Savarit distillation
3. Batch binary distillation
4. Interactive graphical flowsheet preparation
5. Steady-state material balancing simulator
6. Catalytic tubular reactor simulation
7. Numerical integration using Simpson's rule
8. Solution of linear systems using LU decomposition
9. Solution of a single nonlinear equation by half-interval and Newton's methods
10. Solution of systems of n nonlinear design equations in m variables by Newton-Raphson iteration
11. Solution of initial value ODE systems by a 4th-order Runge-Kutta method
12. Linear regression
13. Nonlinear regression (one nonlinear parameter)

Four modules (1, 2, 3, and 5) have been extensively tested by a total of about 200 students in three courses in the Chemical Engineering Department at the University of Michigan during the fall and winter terms. Student response has been quite positive so far.

In addition, User and Module Writer Manuals have been written (an Instructor's Manual is in preparation); and a variety of module preparation

and utility programs (e.g., a graphics package) have been written and debugged.

We have arranged to have the system tested with some of the modules at three other chemical engineering departments within the next month or two, after which the system and modules will be improved as seems appropriate.

Our plans are to make the MicroCACHE system and the existing prototype modules available to Chemical Engineering Departments having the appropriate equipment (and interest) some time during the fall of 1983. The precise distribution mechanism will probably be determined at the June meeting of the CACHE Trustees.

We are currently seeking additional funding to prepare the MicroCACHE system and lessons for delivery on other microcomputers (the IBM PC is the most likely first target machine at this point) and to promote the writing of educational modules by chemical engineering faculty. The MicroCACHE effort is a project of the CACHE Personal Computing Task Force.

LIST OF INDUSTRIAL CONTRIBUTORS TO CACHE

The following companies have contributed financial support to specific CACHE activities during 1981-83:

Chiyoda Chemical Engineering and Construction Company
Digital Equipment Company (DEC)
DuPont Committee on Educational Aid
EXXON Research & Engineering Company
The Halcon SD Group, Inc.
Monsanto Fund, Monsanto Company
Olin Chemicals Corporation
Process Simulation Intl
Shell Companies Foundation
Tennessee Eastman Co.
Weyerhaeuser Company

LIST OF CHEMICAL ENGINEERING DEPARTMENTS SUPPORTING CACHE

CACHE recently concluded a solicitation of universities for funds to carry out on-going CACHE activities and to provide seed money for new projects. Departments providing support for the 1982-84 period, as well as the 1981-83 period, are as follows:

1982-1984

University of Arizona
Auburn University
University of California, Davis
University of California, Santa Barbara
Clemson University
Colorado School of Mines
University of Colorado
Cornell University
Georgia Institute of Technology
University of Houston
Howard University
Illinois Institute of Technology
Iowa State University
University of Iowa
Johns Hopkins University
Kansas State University
University of Kentucky
Lafayette College
Lehigh University
Louisiana State University
University of Maryland
University of Michigan
University of Minnesota
Mississippi State Univ
University of Nevada, Reno
New Jersey Institute of Technology
City College of New York
University of North Dakota
Northeastern University
Northwestern University
Ohio State University
University of Pittsburgh
Princeton University
Purdue University
Rensselaer Polytech Institute
Rose-Hulman Institute of Technology
South Dakota School of Mines
University of South Florida
University of Southwestern Louisiana
Virginia Polytechnic Institute and State University
Washington University
West Virginia College of Graduate Studies
West Virginia Institute of Technology
West Virginia University
Widener University
University of Wyoming
University of Waterloo

1981-1983

University of Alabama
Brigham Young University
Bucknell University
California State Poly Univ, Pomona
University of California, Davis
University of California, Santa Barbara
California Institute of Technology
Carnegie-Mellon University
Case Western Reserve University
University of Cincinnati
Clarkson College of Technology
Cleveland State University
University of Dayton
University of Delaware
University of Florida
Kansas State University
Lamar University
Michigan State University
University of Nebraska
Polytech Institute of New York (Brooklyn)
Ohio University
University of Oklahoma
Oklahoma State University
Oregon State University
University of Pennsylvania
Pennsylvania State University
University of Rhode Island
University of Rochester
Stevens Institute of Technology
University of Tennessee
University of Texas

Texas A & M University
Texas Tech University
University of Toledo
University of Tulsa
University of Utah
University of Virginia
University of Washington
Wayne State University
University of Wisconsin, Madison
Worcester Polytechnic Institute
Yale University
Youngstown State University
University of Alberta
University of Calgary
University of New Brunswick
Nova Scotia Technical College
Universidad de las Americas
Universidad de Concepcion
Eidgenossische Technische Hochschule (E.T.H.)
Universidad Nacional del Sur

CACHE TASK FORCES

Most of the work done by CACHE is through the efforts of its task forces. Current task forces and chairmen are as follows. Please note the newly formed task force on process design case studies. Those wishing to work on task forces are encouraged to contact the designated chairman.

Task Force	
CACHE Conferences:	Professor Richard S. H. Mah Northwestern University
Data Management:	Professor R. L. Motard Washington University
CHEMI Continuation:	Professor D. M. Himmelblau University of Texas, Austin
Graphics:	Professor G. V. Reklaitis Purdue University
Large-Scale Systems:	Professor J. D. Seader University of Utah
Personal Computing:	Professor H. S. Fogler University of Michigan
Microcomputers:	Professor P. R. Rony Virginia Polytechnic Institute and State University
Process Design Case Studies:	Professor M. Morari University of Wisconsin-Madison
Computer-Based Instruction:	Professor M. Cutlip University of Connecticut (On leave at Univ of Cambridge)

CACHE COMPUTER PROGRAMS FOR CHEMICAL ENGINEERING STILL AVAILABLE

In 1972, CACHE published seven volumes of "Computer Programs for Chemical Engineering." The volumes covered the following areas: Stoichiometry, Kinetics, Control, Transport, Thermodynamics, Design, and Stagewise Computations. Each volume contains descriptions and listings of from 11 to 24 tested FORTRAN programs prepared by eminent chemical engineering educators. The programs have proven useful for homework problems, classroom demonstrations, design laboratories, and process simulation. The seven volumes are still available individually at prices ranging from $12.95 to $14.95, and as a complete set at $89.95. Complete information on the volumes is available from the current publisher:

Sterling Swift Publishing Company
P. O. Box 188
Manchaca, TX 78652

AICHEMI MODULAR INSTRUCTION SERIES AVAILABLE

AIChE is publishing one volume per year of each of the AICHEMI Modular Instruction Series listed below. The series were prepared by CACHE under the direction of Professor Ernest J. Henley of the University of Houston and William A. Heenan of Texas A and I University.

Series

A. **Process Control:** T. F. Edgar, Editor
B. **Stagewise and Mass Transfer Operations:** E. J. Henley, Editor
C. **Transport:** R. J. Gordon, Editor
D. **Thermodynamics:** B. M. Goodwin, Editor
E. **Kinetics:** H. S. Fogler and B. L. Cyrnes, Editors
F. **Material and Energy Balances:** D. M. Himmelblau, Editor

The modules were designed to be used for outside study, special projects, entire university courses, review courses, correspondence courses, continuing education courses, or to provide new and timely material that can supplement other courses. A tentative outline listing titles and authors of all modules appears in the volume distributed to all chemical engineering departments. The volumes are available from:

Publications Department, AIChE
345 East 47 Street
New York, NY 10017

by single volume or by subscription.

PERSONAL COMPUTER USERS AND SOFTWARE

Professor Bruce Finlayson has a list of personal computer users in Chemical Engineering education giving the type of machine, area of interest, and available software. If you would like a copy of the list and/or would like to be added to it, fill out the form at the end of this Newsletter and return it to him at the Department of Chemical Engineering, BF-10, University of Washington, Seattle, WA 98185.

CACHE REAL-TIME COMPUTING MONOGRAPHS BEING CLOSED OUT

MONOGRAPHS BEING CLOSED OUT AT $15/set + postage and handling

In 1977, the CACHE Real-Time Computing Task Force, under the direction of Professor Duncan Mellichamp, prepared eight monographs on the following topics in Real-Time Computing:

MONOGRAPH I **AN INTRODUCTION TO REAL-TIME COMPUTING**

0. Digital Computing and Real-Time Computing Digital Computing (Mellichamp)
1. The Structure of Real-Time Systems (Mellichamp)
2. An Overview of Real-Time Programming (Mellichamp)

MONOGRAPH II **PROCESSING, MEASUREMENTS, AND SIGNAL PROCESSING**

3. Processes and Representative Applications (Edgar)
4. Measurements, Transmission, and Signal Processing (Wright)

MONOGRAPH III **INTRODUCTION TO DIGITAL ARITHMETIC AND HARDWARE**

5. Representation of Information in a Digital Computer (Fisher and Seborg)
6a. Digital (Binary) Logic and Hardware (Engelberg and Howard)

MONOGRAPH IV **REAL-TIME DIGITAL SYSTEMS ARCHITECTURE**

6b. Digital Computer Architecture (Engelberg and Howard)
7. Peripheral Devices and Data Communications (Rudd)
8. Digital Computer/Process Interfacing (Hughes)

MONOGRAPH V **REAL-TIME SYSTEMS SOFTWARE**

9. Assembly Language Programming (Fisher)
10. Utility or Systems Software (White)
11. Multitask Programming and Real-Time Operating Systems (Wright)

MONOGRAPH VI **REAL-TIME APPLICATIONS SOFTWARE**

12. Real-Time BASIC (Mellichamp)
13. Real-Time FORTRAN (White)
14. Control-Oriented Languages (Smith)

MONOGRAPH VII **MANAGEMENT OF REAL-TIME COMPUTING FACILITIES**

15. System Justification, Selection, and Installation (Smith)
16. System Operations Management and Program Documentation (McCarthy and Weaver)

MONOGRAPH VIII **PROCESS ANALYSIS, DATA ACQUISITION, AND CONTROL ACQUISITION, AND ALGORITHMS**

A. Process Analysis and Description (Edgar)
B. Digital Computer Control and Signal Processing Algorithms (Edgar and Wright)

These monographs are intended for use in lab courses, in self-study, and by real-time users at all levels because they contain many detailed examples. The monographs have been in heavy demand, particularly due to the trend towards use of real-time computing in the undergraduate laboratory. The monographs are being used as texts in a numer of universities and are available as single volumes at $3.75. Complete sets are now being closed out at $15.00, plus postage and handling from

Professor Brice Carnahan
CACHE Publications Committee
Chemical Engineering Department
Dow Bldg, North Campus
University of Michigan
Ann Arbor, MI 48109

An order form appears at the end of this Newsletter.

HEAT EXCHANGER NETWORK SYNTHESIS PROGRAM

by Manfred Morari

The program RESHEX (RESilient Heat EXchanger network synthesis) was developed at the University of Wisconsin with three objectives in mind:

1) To serve as a tool for continuing research in the area of heat exchanger network synthesis.

2) To serve as an educational aid for undergraduate and graduate students or anybody else learning new synthesis techniques.

3) For anybody applying the techniques on a routine basis to greatly reduce the drudgery of hand calculations and graphical procedures.

The synthesis method for streams with fixed properties is based on the problem table analysis by Linnhoff and Flower. The procedure used to handle constraints on the allowed matches is described by Cerda, Westerberg, Linnhoff, and Mason. For the case that possible variations in the flowrates and inlet temperatures are to be taken into account during the synthesis, the techniques described by Marselle, Morari, and Rudd, and Saboo and Morari have been implemented. The program is written in VAX-11 FORTRAN (based on FORTRAN 77 (ANSI X3.9-1978) for a VAX11/780 computer using a VAX/VMX V2.3 Operating System.

FEATURES

1. The program is interactive. The user is asked for data or for selection of appropriate options through simple, unambiguous questions.

2. The program is very "friendly." The user can easily correct mistakes made in entering data.

3. The data can be stored and read from a file in order to simplify the development and evaluation of alternative designs.

4. Various segments of the program are independently accessible. This makes it ideal for use in iterative design procedures.

The price for the program is $200 ($180 for departments listed on page 11 that support CACHE).

For more information, write:

Professor Manfred Morari
Department of Chemical Engineering
University of Wisconsin
1415 Johnson Drive
Madison, WI 53706

NEW REPORT

"AN INTRODUCTION TO THE USE OF MATHEMATICAL SOFTWARE FOR ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS"

Major strides have been made during the past decade in the development of software for the computer integration of ordinary and partial differential equations (ODE/PDE). The result has been a body of software, generally termed "mathematical software," based on algorithms designed specifically for the computer solution of large, nonlinear ODE/PDE systems. For example, the numerical integration of systems of several thousand ODEs or sets of 25 or more one-dimensional nonlinear PDEs is now commonplace. Beyond this, mixed ODE/PDE systems which frequently occur in scientific and engineering applications can be accommodated by the numerical method of lines. This approach can also be readily extended to the solution of algebraic/ODE/PDE systems.

While these advances have been documented in a spectrum of journals and advanced books, an introductory account of these developments was not available until the appearance of this new report. Thus the nonexpert (e.g., the scientist or engineer who has a large, difficult problem in ODE/PDEs and who does not wish to spend the time required to learn the necessary numerical analysis and computer programming to generate a solution by writing a program) did not have an introductory source of information for the use of ODE/PDE software.

This report is designed to fill this need. Example applications are presented in detail illustrating how to assemble programs for ODE/PDE systems, using available, quality mathematical software. The 310-page report is available for $50 (check payable to Lehigh University) and contains complete FORTRAN listings of the software and example programs. All of the coding listed in the report is available on nine-track tape at nominal cost. The table of contents for the report is listed below.

Inquiries and orders for the report and a tape copy of the software should be directed to:

Professor William E. Schiesser
Department of Chemical Engineering
Whitaker Laboratory No. 5
Lehigh University
Bethlehem, PA 18015
(215) 861-4264

Table of Contents

CACHE MONOGRAPH SERIES IN REAL-TIME COMPUTING

TO: Brice Carnahan, Chairman
CACHE Publications Committee
Chemical Engineering Department
University of Michigan
Ann Arbor, MI 48109

Please send me the following monographs at $3.75 per volume or $15.00 per complete set:

Monograph	No. Copies	Cost	Total
I. "An Introduction to Real-Time Computing			
II. "Processing, Measurements, & Signal Processing			
III. "Introduction to Digital Arithmetic and Hardware"			
IV. "Real-Time Digital Systems Architecture"			
V. "Real-Time Systems Software"			
VI. "Real-Time Applications Software"			
VII. "Management of Real-Time Computing Facilities"			
VIII. "Process Analysis, Data Acquisition, and Control Algorithms			
Full Set			
Subtotal			
Add 10% for handling			
Total remittance			

Name: _____

Address: _____

_____

_____

(City) (State) (Zip)

Make check payable to CACHE Corporation.

- -

FLOWTRAN BOOKS

TO: ULRICH'S BOOKSTORE
Attention: E. Bundy
549 East University Avenue
Ann Arbor, Michigan 48109

Please send me:

No. of copies __ FLOWTRAN SIMULATION - AN INTRODUCTION, 2nd Edition, by J. D. Seader, W. D. Seader, and A. C. Pauls $13.95 each

No. of copies __ EXERCISES IN PROCESS SIMULATION USING FLOWTRAN, 2nd Edition, Edited by J. P. Clark, T. P. Koehler, and J. T. Sommerfeld $11.95 each

No. of copies __ CACHE USE OF FLOWTRAN ON UCS, 2nd Edition, by R. R. Hughes and L. T. Biegler $2.95 each

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

Name: _____

Address: _____

_____

_____

(City) (State) (Zip)

Make check payable to Ulrich's Bookstore.

PPDS MANUAL

TO: Brice Carnahan, Chairman
CACHE Publications Committee
Chemical Engineering Department
University of Michigan
Ann Arbor, MI 48109

Please send me:

No. of Copies INTRODUCTION TO CACHE VERSION OF PHYSICAL PROPERTY DATA SERVICE

_____ @ $4.95/ea = __________

Add 10% for handling __________

Total remittance __________

Name: ______________________________

Address: ______________________________

____

____

(City) (State) (Zip)

Make check payable to CACHE Corporation

- -

HAND-HELD PROGRAMMABLE CALCULATORS by KROESSER

To: Brice Carnahan, Chairman
CACHE Publications Committee
Chemical Engineering Department
University of Michigan
Dow Bldg, North Campus
Ann Arbor, MI 48109

Please send me ____ copies of "Hand-Held Calculators: A Review of Available Programs to Chemical Engineering Education" by F. William Kroesser

@ $2/ea = ____ + 10% for handling = _____ : **Make ck payable to CACHE Corporation**

Name: ______________________________

Address: ______________________________

____

____

(City) (State) (ZIP)

PERSONAL COMPUTER USERS AND SOFTWARE INFORMATION

Return to:
Professor Bruce A. Finlayson
Department of Chemical Engineering
BF-10
University of Washington
Seattle, WA 98195

Name:_____

School:_____

How many micros do you have available, and type?

_____

_____

_____

Dept: _____

College: _____

University: _____

Which of the following areas are you interested in?

____ Data Acquisition
____ Control
____ Thermo and Physical Properties
____ Databases
____ Computer-Aided Instruction
____ Simulation
____ Design tools; appl._____

_____

- -

CACHE/CAST SESSION REPLY

Return to:
Professor Peter R. Rony
CACHE/CAST Chairman
Department of Chemical Engineering
Virginia Polytechnic Institute & State University
Blacksburg, VA 24061

Responding Individual:_____

University: _____

A representative would like to attend the CACHE/CAST Session ____

A potential speaker from our department is

_____,

who would be interested in speaking on the following topic: _____

_____