

CACHE NEWS

News About Computers
In Chemical Engineering
Education.

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IN MEMORIAM

William H. Corcoran, Institute Professor of Chemical Engineering at the California Institute of Technology died unexpectedly on August 21, 1982, while vacationing in Hawaii with his wife Martha. Professor Corcoran was one of this country's most important engineering educators, served as President of AIChE, and was due to be President of the Accrediting Board of Engineering and Technology (ABET). He was a member of the National Academy of Engineering and served on the Advisory Committee of CACHE for a number of years. He is survived by Martha; his son, Will, Jr., his daughter, Sally Corcoran Fisher, and five grandchildren. Professor Corcoran had a broad influence on chemical engineering and will be greatly missed by his colleagues and friends.

FOCAPD-83 CONFERENCE

Plans are almost complete for 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 in Colorado. The conference is being sponsored by the CAST (Computers and System 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:

**"Systems in Engineering Design -
Progress in the Last Five Years"**

Session I: Chairman, Jerry L. Robertson
EXXON Research & Engineering

"Industrial and Academic Overview"
Roger Sargent,
Imperial College, London

Session II: Chairman, Theodore L. Leininger
DuPont Company

"Computer Science Aspects"
(speakers to be determined)

Session III: Chairman, Warren D. Seider
University of Pennsylvania

"Computational Algorithms"
Gordon Bradley, Naval
Post Graduate School,
Monterey, California

Session IV: Chairman, Joseph Boston
ASPENTech

"Physical Properties for Design"
John P. O'Connell,
University of Florida

Session V: Chairman, Rodolphe L. Motard
Washington University

"Nonsequential Modular Flowsheeting"
John Perkins, Imperial
College, London
Lorenz Biegler, Carnegie-
Mellon University

Session VI: Chairman, Richard S. H. Mah
Northwestern University

"Design of Batch Processes"
G. V. Reklaitis, Purdue
University
Harold N. Gabow, Computer
Science Dept, University of
Colorado

Session VII: Chairman, Bruce A. Finlayson
University of Washington

"Complex Single Unit Design"
Warren E. Stewart,
University of Wisconsin
H. H. Klein, JAYCOR,
San Diego, California

Session VIII: Chairman, Cameron M. Crowe
McMaster University

Contributed Papers (see Call for Papers
at the end of this Newsletter)

Session XI: Chairman, George Stephanopolous
National Technical University

"Operability in Design"
Ignacio Grossmann,
Carnegie-Mellon University
Manfred Morari,
University of Wisconsin

The above meeting program was developed by Professor Westerberg, Dr. Chien, and the Session Chairmen in conjunction with an advisory committee consisting of:

Coleman B. Brosilow
Case-Western Reserve University

Brice Carnahan
University of Michigan

Dwight L. Johnston
Shell Development Co.

John M. Prausnitz
University of California, Berkeley

John H. Seinfeld
California Institute of Technology

Vern Weekman, Jr.
Mobil Tyco Solar Energy Corporation

Ex-Officio Members (FOCAPD-80 Organizers)
Richard S. H. Mah,
Northwestern University

Warren D. Seider
University of Pennsylvania

Snowmass is a spectacular resort located high in the Colorado Rockies, just 20 minutes away from Aspen. At Snowmass, the air is clear and the sunshine warm. The mountain valley is lush with aspen and wild flowers. Snowmass has many fine shops and restaurants, and recreation facilities include ecology tours, nature walks, hiking, fishing, horseback riding, chairlift rides, white-water rafting, swimming, tennis, and golf.

To encourage active participation and discussion at the conference, the number of attendees will be limited, and selection will be made on the basis of involvement in the field of computer-aided process design and analysis. If you are interested in attending the conference and have not already responded to a brochure that was mailed out in August, 1982, please complete the "Form for Further Information about FOCAPD-83" at the end of this newsletter.

The fee for the conference will be \$425 and will include a copy of the proceedings, registration, the reception on Sunday evening, and the banquet on Thursday evening.

Arrangements have been made for single- and double-room lodge accommodations available at the Silver Tree/Eldorado at \$40 per night, double or single occupancy. Thus, the total room cost will be the same whether occupied as a single or double. All rooms have two beds, and a continental breakfast is included in the room rate.

Condominiums, ranging from studio to multiple-bedroom units with kitchens, will be available for families desiring larger accommodations. Detailed information on condominiums, including rates, will be sent to those submitting the "Form for Further Information about FOCAPD-83."

**THIRD CACHE SHORT COURSE ON
MICROCOMPUTER INTERFACING/PROGRAMMING:
GRADUATE STUDENTS TO PARTICIPATE FOR
THE FIRST TIME**

The third CACHE short course on microcomputer interfacing/programming, co-sponsored by the University of Pennsylvania, Department of Chemical Engineering, will be held on the University of Pennsylvania campus, Philadelphia, PA, from Thursday morning, January 6, through late Monday afternoon, January 10, 1983. A one-day introduction to basic concepts of digital electronics followed by a four-day introduction to microcomputer programming (machine code, assembly language) and microcomputer interfacing will be given by Dr. Peter Rony, CACHE Trustee and Professor of Chemical Engineering at Virginia Polytechnic Institute and State University. The hands-on short course will permit you to wire simple digital circuits using digital integrated circuits (gates, latches, counters, decoders, three-state buffers, etc.); interface device decoder, microcomputer input, microcomputer output, and interrupt circuits to an 8080A-based microcomputer; and write and test input/output device driver routines. Four hours of lecture and four hours of laboratory will be provided each day. No background is required other than a knowledge of Ohm's law. For further details, please see either the September 1981 (No. 13) or April 1982 (No. 14) issue of CACHE News.

The number of participants is limited to two per microcomputer station, or a total of 18 participants. Preference will be given to full-time faculty members at Departments of Chemical Engineering. We would be delighted for PhD-level graduate students in chemical engineering to attend if space is available. Selection of both faculty and graduate student participants will be done on a first-come, first-served basis.

If you wish to participate, please send a letter immediately to Dr. Peter R. Rony, Dept of Chemical Engineering, Virginia Polytechnic Institute & State University, Blacksburg, VA 24061 [(703) 961-6370]. You will then receive details of the short course housing, which is being arranged at the writing of this notice. The course fee will be \$125, which includes three or four books, equipment rental, and your pro-rata share of Dr. Rony's travel and lodging expenses. Any excess course fees collected will be refunded to each participant. The fee is payable at the start of the short course.

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 in machine language 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 through CACHE.

CACHE will initiate this new FLOWTRAN project at the University of Utah by preparing for distribution a load module for the UNIVAC 1008 and 1100 series of computers. As a current or former user of FLOWTRAN, you may be interested in preparing a load module for your particular type of machine if it is other than UNIVAC. Those who are approved by Monsanto to prepare a load module for CACHE will be permitted to keep a copy of it at no charge but will be required to return to CACHE all FLOWTRAN source code received or generated. Those departments that order load modules prepared by others will be subject to a moderate cost and to approval by Monsanto Company.

FLOWTRAN consists of approximately 160 subroutines and 60,000 lines of FORTRAN code and data, including comment statements, data files, and test problems. Past experience at Monsanto indicates that it will not be difficult to prepare a load module, but it will be advisable to obtain assistance from your computer center.

Twenty-three departments have already indicated interest in the FLOWTRAN load modules in response to a letter sent to all departments on August 19, 1982.

If you are interested in assisting CACHE in the preparation of a FLOWTRAN load module on your computer or would like to obtain a load module for your computer and you did not receive the announcement letter and form, please complete and submit the form near the end of this newsletter. All departments desiring to prepare or obtain a FLOWTRAN load module will be required to sign an agreement

with Monsanto and CACHE to use FLOWTRAN only for educational purposes and not for consulting or any other activity.

Complete educational materials are available from CACHE. An order blank is given near the end of this newsletter.

NEW CACHE TRUSTEE

At the July 30 to August 1, 1982, annual meeting of CACHE, **Dr. Irven H. Rinard** was elected as an industrial trustee. Dr. Irven is currently Technical Director - Development in the Technology Division of the Halcon SD Group, Inc. He is in charge of corporate activities in systems engineering including control systems analysis and design, dynamic and flowsheet simulation studies, and computer-control implementation. He is the author of Halcon's in-house Time-Sharing Process Simulation System (TPSS), as well as other programs for process design, simulation, and dynamic analysis. Irven has been with Halcon 19 years. Prior to that, he was employed by the American Cyanamid Company in its Process Analysis Group. He holds ScD and SM degrees in chemical engineering from MIT and a BChE from the University of Delaware. He has been active in the CAST Division of the AIChE for the past six years. Also, he is Adjunct Professor at the Polytechnic Institute of New York, where he teaches process dynamics and control. He is the author of several papers on the subjects of process simulation and control.

NEW CACHE OFFICERS

At the July 30 to August 1, 1982, annual meeting of CACHE, two new officers were elected:

1. **Professor Richard S. H. Mah** of Northwestern University is the new Vice President of CACHE. He was one of the two organizers of the first Conference on Foundations of Computer-Aided Process Design (FOCAPD) held on July 6-11, 1980, at New England College, Henniker, New Hampshire. He was recipient of the AIChE CAST Division's Computing in Chemical Engineering Award in 1981, has served as chairman of the CAST Programming Board, and as secretary of CACHE.

2. **Professor G. V. "Rex" Reklaitis** of Purdue University is the new Secretary of CACHE. He is well known for his research in computer-aided design and has served as Chairman of the CACHE task force on Graphics. He is currently involved in establishing at Purdue an interactive computer graphics laboratory, which was discussed in the last issue of CACHE News.

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 number 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 near the end of this Newsletter.

ASEE SUMMER SCHOOL

The ASEE Summer School was held at the University of California at Santa Barbara during August 1-6, 1982. Areas covered at the Summer School included:

- (1) New Technical Directions in Chemical Engineering
- (2) Expanding Role of Computers in Chemical Engineering Education
- (3) Curricula, Courses, and Laboratories
- (4) Industrial-University Interactions
- (5) Chemical Engineering and Its Interactions with Society
- (6) Chemical Sciences and Chemical Engineering

The Computing Sessions in Area (2) were coordinated by T. F. Edgar, Professor at the University of Texas and President of CACHE. Several CACHE members participated in these sessions. In addition, a session on process dynamics and control curricula was conducted under Area (3) by Professor D. A. Mellichamp of CACHE and Professor D. E. Seborg, both of the University of California at Santa Barbara.

The computing sessions, which were among the most-attended sessions at the school, included:

1. Computer Graphics and Modular Instruction, with demonstrations
G. V. Reklaitis, Y. Arkun,
D. M. Himmelblau, M. Cutlip,
S. I. Sandler, M. Bailey
2. Use of Computers in Teaching Process Design
J. D. Seader, W. D. Seider,
R. S. H. Mah, G. V. Reklaitis,
I. Grossmann, E. J. Henley
3. Personal Computing
B. Carnahan, B. Finlayson
W. Stevens
4. Microcomputers in Chemical Engineering Laboratories
P. R. Rony
5. Teaching of Process Synthesis in Process Design
M. Morari, I. Grossmann

Professors who were unable to attend the summer school, but may be interested in details of any of the topics covered, should write to the professors named above.

STATUS OF ASPEN SIMULATOR

Many professors have expressed interest in obtaining the MIT/DOE ASPEN program for computer-aided design and simulation. ASPEN is written in FORTRAN and consists of the following seven systems:

1) IT (INPUT TRANSLATOR):

Translates user input data into a calling program that is linked with all necessary ASPEN subroutines to run a simulation.

2) SP (SIMULATION PROGRAM):

Carries out any of the following classes of runs:

- A. Simulation
- B. Costing only
- C. Data regression
- D. Generation of data tables

3) DFMS (DATA FILE MANAGEMENT SYSTEM):

Creates, modifies, and prints contents of data banks (e.g., physical property constants)

4) TBS (TABLE BUILDING SYSTEM):

Creates and modifies the System Definition File (SDF), which contains all keywords for input data, names of models and default values for their parameters, etc.

5) SDFRPT (SDF REPORT WRITER)

Prints all or a portion of SDF

6) DMSRUN (DATA MANAGEMENT SYSTEM RUN)

Manages the data system, which utilizes a single array called PLEX

7) IFMS (INSERT FILE MANAGEMENT SYSTEM)

Creates and maintains user-generated files (e.g., input data, blocks of FORTRAN statements, etc.)

The ASPEN project was founded in 1976 at the Massachusetts Institute of Technology and was completed in 1981 with the help of 55 companies and government groups. The program consists of 353,482 lines of FORTRAN code, 170,000 lines of executable FORTRAN code, 27 megabytes of characters, and 1,511 subroutines. The ASPEN source code will soon be available for IBM (CMS, OS), UNIVAC, and

VAX-11/780 computers. If interested, contact:

Margaret Butler
National Energy Software Center
9700 South Cass Avenue
Argonne, IL 60439
(312) 972-7250

An ASPEN User's Group has been formed. If interested, contact:

Leonard A. Fabiano
ARCO Chemical Co.
3801 West Chester Pike
Newtown Square, PA 19073
(215) 359-2000

ASPEN PLUS AVAILABLE OVER EDUNET

Faculty members, staff, and students at colleges, universities, and non-profit institutions now have access to ASPEN PLUS, a state-of-the-art chemical process simulator through EDUNET, an international computing network for higher education and research, sponsored by EDUCOM.

ASPEN PLUS is a commercial, maintained version of the ASPEN Process Simulator originally developed at MIT. Using English-like terminology and flowsheet conventions, non-programmers can perform steady-state material balances, estimate equipment costs, and carry out economic evaluations. ASPEN PLUS provides for a wide variety of equipment and processes to be simulated in a number of areas including petrochemical plants, environmental control processes, and distillation systems.

Under the agreement between EDUNET and ASPEN Technology, Inc., ASPEN PLUS will be available on the MIT computer to users at EDUNET member institutions. Provision has also been made for non-members to access ASPEN PLUS through EDUNET as well. It can be accessed through Telenet or TYMNET by making a local call in over 300 U. S. cities. The user will pay only for computer time and storage with no royalty or fee to ASPENTech. For EDUNET members, there will be a monthly storage charge of \$50. The charge for non-members will be \$100/month with a minimum of three months to defray storage and account processing costs. Interactive computing costs for building ASPEN models depend on time of day and resources being used, but typically run \$12-15/hr, including telecommunications costs. Cost for running an ASPEN PLUS simulation again depends on

time of day and size of the model but should be in the range of \$10-30/run. These costs compare very favorably with those of commercial service bureaus and represent a considerable savings to the educational and non-profit user.

Billing for computer services, account initiation, and setup, as well as administrative and user-support services are provided by the EDUNET staff. In addition, EDUNET provides help in locating and accessing a range of other resources at its supplier institutions, including CRAY supercomputing, powerful database management systems, an array of economic mail and conference facilities, and numerous other specialized programs at its 17 supplier institutions.

A series of one-day "Introduction to ASPEN PLUS" seminars have been scheduled for the first two weeks of November in New York, Chicago, Atlanta, Houston, Denver, and San Francisco. Longer, in-depth seminars on ASPEN PLUS and particular applications are also scheduled through the year. Partial tuition scholarships for the longer seminar as well as educational discounts on ASPEN PLUS documentation are available. To find out if your institution is a member of EDUNET or for further information on ASPEN PLUS or any other EDUNET resources, call the EDUNET hot-line at (609) 734-1878.

MATHEMATICAL SOFTWARE LIBRARY

Professor William E. Schiesser, a CACHE Trustee from Lehigh University, has assembled a mathematical software library for applications to algebraic equations, partial differential equations, and ordinary differential equations including stiff systems. Bill can provide copies of these routines or information on how they can be obtained. His library is as follows, where routines marked with an asterisk are not yet in the library but are being considered for inclusion.

NAME	AUTHOR(s)	DESCRIPTION/USE
DESTEP	Shampine and Gordon	Explicit, multi-step integrator for initial-value ODEs
RKF45	Forsythe, Malcom, and Moler	Explicit, fifth-order, variable-step Runge-Kutta integrator for initial-value ODEs
EPISODE	Byrne and Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with full Jacobian matrix and step-size adjustment for steep fronts
EPISODEB	Byrne and Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with approximately banded Jacobian matrix and step-size adjustment for steep fronts
LSODE	Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with full or approximately banded Jacobian matrix
LSODI	Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with implicit banded coupling of the temporal derivatives; this form of coupling occurs in the use of weighted residuals and finite elements
LSODES	Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with sparse Jacobian matrix; the sparse matrix calculations are performed by the Yale sparse matrix code
LSODIS*	Sherman	A combination of LSODI and LSODES for implicitly coupled ODEs with sparse matrix processing of the Jacobian matrix
LSODA	Hindmarsh	Variable-order, variable-step integrator with automatic switching between stiff and non-stiff options
LSODAR	Hindmarsh	Implicit, variable-order, variable-step integrator for mixed algebraic/stiff differential systems with automatic root finding for the algebraic equations
IMP	Stutzman and Babcock	Implicit, variable-step integrator based on the algorithm by Brandon with sparse matrix processing of the Jacobian matrix
DGEAR	IMSL	Integrator for initial-value ODEs based on Adams predictor-corrector for non-stiff systems or Gear's BDF methods for stiff systems
DREBS	IMSL	Integrator for non-stiff initial-value ODEs based on an extrapolation method
DVERK	IMSL	Integrator for non-stiff initial-value ODEs based on the Runge-Kutta-Verner fifth- and sixth-order methods

STIFFZ	Carver and Dissinger	Implicit, variable-order, variable-step integrator for stiff differential systems with full, banded, or sparse Jacobian matrix structure; the sparse matrix option is based on the Harwell sparse matrix code by Reid
GEARBI	Hindmarsh	Implicit, variable-order, variable-step integrator for stiff differential systems with block iterative processing of the Jacobian matrix; this integrator has particular utility for the numerical method of lines integration of multidimensional PDEs
DASSL*	Petzold	Implicit integrator for mixed algebraic/stiff differential systems
DASP3	Soderlind	Runge-Kutta-BDF code for partitioned stiff ODEs and mixed algebraic/stiff differential systems
ASIRK	Seider	Semi-implicit Runge-Kutta integrator for stiff ODEs with adjustment of the time step by estimation of the largest temporal eigen-value
DEPAC*	Shampine	A collection of three user-selected algorithms for stiff and non-stiff problems: 1) DERKF - a Runge-Kutta-Fehlberg explicit integrator 2) DEABM - an Adams-Bashforth-Moulton explicit integrator 3) DEGRK - combination of a Runge-Kutta-Fehlberg non-stiff integrator and a Rosenbrock semi-implicit Runge-Kutta stiff integrator with automatic switching between the two integrators
MRK* STRIDE BLEND DIRK STINT	Gaffney	Collection of codes based on implicit and semi-implicit Runge-Kutta methods of varying order and stability
SIRK* LSTIFF	Crosbie	Two codes based on semi-implicit Runge-Kutta methods of varying order and stability
ATSMCC*	Corliss	Automatic Taylor series by Morris, Chang, and Corliss, an integrator based on the Taylor series for stiff differential systems
MAKSIM	Carver	Implicit, variable-order, variable-step integrator for stiff differential systems with front-end processor for ODEs arising in mass-action kinetics
SUPPORT	Scott	Routines for the solution of boundary-value ODEs by a variety of methods, e.g., shooting, superposition-orthonormalization, quasilinearization
COLSYS	Ascher	Integrator for boundary-value ODEs based on spline collocation; special case integration of initial-value ODEs is possible
DVCPR	IMSL	Integrator for boundary-value ODEs based on a variable-order, variable-step finite difference method with deferred corrections
DTPTB	IMSL	Integrator for boundary-value ODEs based on a multiple shooting method

FORSIM	Carver	Solution of ODE/PDE systems by the numerical method of lines; includes a variety of explicit and implicit integrators for initial-value ODEs and a variety of approximations for PDE boundary-value (spatial) derivatives in one to three dimensions
PDECOL	Sincovec and Madsen	Solution of one-dimensional PDEs by the numerical method of lines; approximation of the PDE boundary-value (spatial) derivatives by polynomials evaluated through collocation
DSS/2	Schiesser	<p>Solution of ODE/PDE systems by the numerical method of lines; includes:</p> <p>14 explicit Runge-Kutta integrators, orders two to five, with one-, two-, and three-term error estimates</p> <p>Implicit, variable-order, variable-step integrator with full, banded, and sparse matrix processing of the ODE Jacobian matrix</p> <p>Central and upwind polynomial approximations of the boundary-value (spatial) derivatives in PDEs in one, two, and three dimensions</p> <p>Variable and adaptive grid approximations of the boundary-value derivatives in one-dimensional PDEs</p> <p>Interface between selected integrators for initial-value ODEs, e.g., LSODE, LSODES, and DSS/2 PDE differentiation routines; the user can then synthesize a numerical method of lines code</p>
MOLID	Hyman	Method of lines routines for one-dimensional PDEs with particular application to hyperbolic PDEs written in conservation form
DYLA*	Miller and Gelinas	Method of lines code for PDEs based on the moving finite element method; one- and two-dimensional PDEs with steep moving fronts and shocks can be accommodated
DPDES	IMSL	Routine for a system of one-dimensional PDEs based on the numerical method of lines with cubic Hermite polynomials
DBCEVL	IMSL	Routine for mixed partial derivatives from bicubic splines
DCSEVU	IMSL	Routine for first- and second-order derivatives by cubic splines
NCSPLE	Hu and Schiesser	Modified cubic splines for the calculation of first-, second-, and third-order derivatives with user-defined end conditions for the dependent variable and its first-, second-, and third-order derivatives
REACOL	Finlayson	Collocation analysis of selected parabolic PDEs with application to chemical reactors
REACFD	Finlayson	Finite difference analysis of selected parabolic PDEs with application to chemical reactors
LINPACK	Dongarra, Bunch, Moler and Stewart	Library of routines for linear algebra and, in particular, application to linear algebraic equations with coefficient matrices of varying structure

MINPACK	Garbow, Hillstom, and More	Library of routines for the direct and least-squares solutions of systems of nonlinear algebraic and transcendental equations
PITCON*	Rheinboldt and Burkardt	Routine implementing a locally parameterized continuation process for the solution of systems of nonlinear algebraic and transcendental equations
YALE	Eisenstat and Schultz	System of routines for the solution of linear algebraic equations with arbitrary, sparse coefficient matrix

**PROCESS TROUBLESHOOTING EXERCISES
OF IAN DOIG**

Professor Ian D. Doig, of the School of Chemical Engineering and Industrial Chemistry, University of New South Wales in Australia, recently spent six months with Professor David M. Himmelblau, CACHE Trustee, at the University of Texas at Austin. While there, Professor Doig extended software and student and instructor exercise manuals associated with a process-troubleshooting exercise program that he has developed.

The exercises use a detailed simulation of all components of a processing plant (including piping and valves). Various malfunctions, each producing a significant disturbance in a limited set of measurements of overall process performance, are modelled into the simulation to produce a complete stream/properties matrix for each process fault.

Students begin each exercise set by studying the limited set of measurements and following a strategy of:

- 1) Identifying the problem
- 2) Postulating valid causes for the observed behavior
- 3) Specifying tests/measures of flowrate, analyses, temperature, pressure and/or pressure drop which, together with local mass, energy and/or pressure balancing will confirm or deny particular postulated causes until they have located and identified the cause of the malfunction.

Each measurement called under item 3 above views a notional dollar charge, and par values have been established for each malfunction exercise. No reported measurement is exact: a random number selector and Gaussian subroutine adds (+ or -) a typical measurement error to each exact value before reporting it to the student. Two processes have been simulated;

a hydrocarbon chlorination process involving two reactors in series with an absorber removing HCl from recycled chlorine, and a two-column distillation set.

Professor Doig's program is now being extensively tested at the University of Texas and is expected to be ready for distribution by CACHE at the end of 1982 or early in 1983.

**OPEN HOUSE FOR CACHE REPRESENTATIVES
AT AIChE LOS ANGELES MEETING**

CACHE is pleased to invite CACHE representatives or their designated alternates to attend an open house in the Santa Barbara A Room of the Bonaventure Hotel in Los Angeles from 5 to 7 p.m. on Wednesday, November 17, 1982, in connection with the Los Angeles AIChE meeting.

CACHE will have informative displays of their current projects and products and will provide cheese, snacks, and various beverages.

**AIChE LOS ANGELES MEETING
OPTIMIZATION PROGRAM**

by G. V. Reklaitis

The Los Angeles meeting program will include a two-session symposium reviewing the state-of-the-art of large-scale optimization methodology. The speakers include well-known experts in nonlinear programming techniques as well as chemical engineering applications specialists. The detailed symposium program is listed below. A third companion session will focus on applications involving entire plant optimization. Selected papers from the three sessions will appear as a special issue of Computer and Chemical Engineering early in 1983.

SYMPOSIUM

Sponsored by the Computers in Management and
Information Process Area (C)
National Program Committee, Group #10
CAST Division

Gintaras Reklaitis, Chairman
I. Grossmann, Vice Chairman

THE STATUS OF LARGE-SCALE OPTIMIZATION I

Title; Author(s); Abstract of Presentation

"Large-Scale Unconstrained Optimization";

David F. Shanno; This paper concerns recent developments in methods for minimizing unconstrained nonlinear functions with many variables. Recent theoretical results and computational experience with truncated Newton methods and Buckley's variable storage preconditioned conjugate gradient method will be stressed.

"Large-Scale Mathematical Programming Systems";

John A. Tomlin; This survey covers the state-of-the-art of the large-scale mathematical programming systems for solving problems which can be modelled using linear programming or its extensions, such as mixed-integer and some types of nonlinear programming. Such models occur frequently in chemical engineering and other types of process, manufacturing, and distribution applications.

"Large-Scale Convex Quadratic Programming";

Jong-Shi Pang; This paper surveys various methods for solving convex quadratic programming problems. The discussion is centered on (i) the unification of several classes of finite methods, (ii) recent developments of iterative methods, and (iii) the numerical implementation of several finite and iterative methods for large-scale problems.

THE STATUS OF LARGE SCALE OPTIMIZATION II

"Large-Scale Nonlinear Programming"; Leon Lasdon; The algorithms most suitable for solving large nonlinear programs appear to be successive linear programming, successive quadratic programming, and generalized reduced gradient methods. This paper will discuss features, software, and computational tests of these methods. The focus will be on aspects pertinent to optimal design and operation of chemical processes.

"Exxon Experience with Large-Scale Linear and Nonlinear Programming Methodology"; Jerome Simon (speaker) and H. M. Azma; A recent study at Exxon was conducted to compare the

performance of our sequential linear programming and sequential quadratic programming codes with reduced gradient technology employed in GRG II and MINOS. The findings indicated that there are application areas in which each has an advantage.

"Large-Scale Applications of Successive Quadratic Programming Methodology";

Arthur W. Westerberg (speaker) and Michael H. Locke; Many chemical engineering optimization problems are characterized by having large numbers of equations and few degrees of freedom. This paper describes a new variation of the Han-Powell algorithm that sets up a QP in only the decision variables. The method has been implemented with ASCEND-II, an interactive equation-based flowsheeting system, where any variable can be selected as the objective and/or constrained arbitrarily.

"An Approach to Large-Scale Nonlinear Programming";

D. R. Heltne (speaker), J. O. Osburn and J. M. Liittschwager; This paper presents an approach to a large-scale GRG algorithm utilizing sparse matrix decomposition. The key to the approach is an algorithm for dynamically ordering the GRG basis matrix into block lower triangular form after a column replacement. The GRG computational improvements come from 1) never computing the complete Jacobian matrix, and 2) reduced computations in the GRG feasibility phase.

"Process Optimization: A Comparative Case Study";

Lorenz T. Biegler (speaker) and Richard R. Hughes; Four recently developed algorithms were tested on a realistic propylene chlorination process simulation. All four are based on successive quadratic programming and interface easily with most sequential modular simulation packages. Using SPAD for simulation, optimal cases were obtained in as few as 29 simulation-time equivalents. The paper includes model details, reactor kinetics, and algorithm performance.

OPTIMIZATION OF ENTIRE PLANT OPERATIONS

"Restrains on Entire Plant Optimization";

D. E. Haskins; The restraints to entire plant optimization are discussed in approximate order of importance: lack of proven incentives, manpower limitations, regulatory control requirements, incomprehensibility, model and objective function inadequacies, and computer resource limitations. Examples of these restraints are presented and directions for future developments are discussed.

"Real-Time Optimization with Multivariable Control is Required to Maximize Profits";

C. R. Cutler; The use of a control computer with real-time capabilities is a necessary condition for optimization of a process. Feedback of the current state of a process is required to adapt models and precisely define physical restraints. Multivariable computer control at constraints is required to realize optimization benefits.

"Business Planning and Optimization of a Refinery/Petrochemical Complex";

N. C. Cilley (speaker) and R. Nedwick; Planning of production and operation is done by optimization of a profit function. Linear models optimize volumetric plans based on market demands, prices, raw material availability, and plant operation condition for each planning period. Nonlinear models for each plant optimize daily operating targets. Specific unit operations have on-line optimization control.

"Computerized Optimization of Complete Process Flowsheets";

T. B. Challand; A user-friendly advanced simulation program combined with a non-linear multi-variable optimization algorithm allows overall optimization of complete process flowsheets. An objective function based on feedstock costs, product values, and utility consumptions is maximized by manipulating selected process variables such as pressure, temperature, and flowrates illustrates a gas processing industry application.

"Simulation and Optimization of a Specialty Chemicals Production Plant";

R. M. Felder (speaker), P. D. Kester and M. M. McConney; An approach to simulation, debottlenecking, optimization, and expansion of plants containing primarily batch processes is described. A commercially available simulation program (GASP-IV) implemented on a specialty chemicals manufacturing plant provides several specific means of substantially increasing productivity and in some cases simply by changing procedures with no required capital expenditures.

**NEW COMPUTER-BASED INSTRUCTION
TASK FORCE**

Recently elected CACHE trustees, Professor Stanley I. Sandler at Delaware and Professor Michael B. Cutlip at Connecticut, have formed a new task force in computer-based instruction (CBI). One of the purposes of this task force will be the dissemination of information on the capabilities of various computer-based instructional systems. This will include a wide range of computers from the Control Data PLATO system to small microcomputers such as the Commodore and the APPLE. Efforts will also be made to distribute information on chemical engineering materials as they become available.

If you would like to become involved with the task force, please contact Professor Michael Cutlip who is currently on sabbatical leave at the Dept of Chemical Engineering, Dow Bldg, North Campus, University of Michigan, Ann Arbor, MI 48109.

CHE MATERIALS AVAILABLE ON PLATO

by Profesor Michael B. Cutlip

Chemical engineering lessons are now available on the Control Data Corporation PLATO educational computer system at over 18 locations throughout the world. Access to these materials requires a CDC PLATO terminal and regular telephone lines for communication.

Stoichiometry Some 19 lessons by Professor Charles Eckert at the University of Illinois, which were demonstrated at the ASEE Summer School, have been created to accompany an introductory course in chemical engineering. These lessons compliment the textbook by Professors Felder and Rousseau and the textbook by Professor Himmelblau. Professor Eckert has used these lessons successfully as additional materials in an otherwise traditional introductory course in chemical engineering. The file names, subject titles, and approximate terminal times are as follows:

Oche1	Material Balances w/o Chemical Reaction (Basic)	40 min
Oche2	Material Balances w/Chemical Reaction (Basic)	75 min
Oche3	Introduction to PLATO	30 min
Oche4	Enthalpy Effects	60 min
Oche5	Total Energy Balance, Steady State, Part 2	80 min
Oche6	Material Balances w/Chemical Reaction (Adv)	55 min
Oche7	Material Balances w/o Chemical Reaction (Adv)	30 min
Oche8	Thermodynamic Diagrams (Basic)	35 min
Oche9	First Law of Thermodynamics, Closed Syst., Part 1	30 min
Oche10	Change-of-Phase Problems	60 min
Oche11	Ideal Gases and Real Fluids, Part 1	85 min
Oche12	First Law of Thermodynamics, Closed Syst., Part 2	85 min
Oche13	Data Analysis	25 min
Oche14	Introduction to Equilibrium Stages	55 min
Oche15	Intro. to Units, Symbols, and Reaction Stoichiometry	70 min
Oche16	Total Energy Balance, Steady State, Part 1	50 min
Oche17	Ideal Gases and Real Fluids II	45 min
Oche18	Unsteady State Material Balances	45 min
Oche19	Unsteady State Energy Balances	40 min

Numerical Analysis Interactive numerical analysis lessons, which were demonstrated at the ASEE Summer School, have been authored by Professor Michael Cutlip at Connecticut and Professor Mordechai Shacham at Ben-Gurion University of the Negev in Israel. These lessons combine existing capabilities of the PLATO system with state-of-the-art numerical methods to provide a convenient simulation package which makes efficient use of interactive graphics in problem solving. An article entitled "A Simulation Package for the PLATO Educational Computer System," which describes these lessons in detail has been published in Computers and Chemical Engineering, Vol. 6, No. 3, pp. 209-218, 1982. Summaries of these three open-ended lessons are given below:

- Ønonlin - Linear/Nonlinear Equation Solver: capable of solving systems of algebraic equations containing up to 6 linear or nonlinear equations
- Ødifeq - Differential Equation Simulator: capable of solving systems of first-order, ordinary differential equations (up to 6 simultaneous equations)
- Øpolreg - Regression/Curve Fitting Routine: capable of fitting a polynomial of up to the 5th order to experimental data.

Future PLATO Lessons Additional chemical engineering materials are currently under development, and a status report will appear in the next CACHE newsletter.

**MICROCOMPUTER TASK FORCE -
ACTIVITIES AND UNIVERSITY CONTACTS**

To meet the growing interest within chemical engineering departments in microprocessors, microcomputer interfacing to laboratory experiments, and microcomputer-based real-time computing, CACHE activities in these areas have been consolidated into a CACHE Microcomputer Task Force, headed by Dr. Peter R. Rony, Virginia Polytechnic Institute and State University, and Dr. Joseph D. Wright, McMaster University and Xerox Research Centre of Canada.

The activities of the task force will include the CACHE short courses on microcomputer programming/interfacing elsewhere announced in this newsletter, the dissemination of information on laboratory experiments in chemical engineering, surveys on microcomputer activities and interests within chemical engineering departments, a CACHE speaker's bureau, and a new idea: "CACHE consultants," chemical engineering faculty with specific expertise with certain types of microprocessors (Z80, 8085, 8080, 6502, 8086, 68000, etc.) and personal computers (IBM, APPLE, Zenith, Radio-Shack, Xerox, etc.) who would consult for other chemical engineering departments for a standard fee established by CACHE.

The CACHE Microcomputer Task Force university contact (see list below) or CACHE representative will soon receive a questionnaire that probes current work in chemical engineering departments with microcomputers or personal computers in laboratory applications such as real-time control, data logging, system timing, sequencing, etc.; the availability of information on such work, including reports, articles, and theses; what can be done to augment the administration perception of the value of such work; and local interest in "CACHE Consultants."

At the recent 1982 ASEE Summer School for chemical engineering faculty (August 1-6, 1982, University of Santa Barbara), CACHE requested a representative from each chemical engineering department to serve as a department contact for the CACHE Microcomputer Task Force. Such a representative would receive announcements of task force activities and would be occasionally requested to participate in surveys. To date, we have the following list

of departmental representatives. If your department is not represented and you would like to serve as our contact because of your interest in the area, please send your name and phone number on your department letterhead to Dr. Peter Rony, Department of Chemical Engineering, Virginia Polytechnic Institute & State University, Blacksburg, VA 24061.

William D. Baasel, Ohio Univ
Dee H. Barker, Brigham Young Univ
Duane D. Bruns, Univ of Tennessee
Eugene V. Cilento, West Virginia Univ
Kenneth A. Debelak, Vanderbilt Univ
Richard W. Freedman, Tulane Univ
Ahmed M. Gadalla, Texas A & M Univ
Bret L. Halpern, Yale Univ
Archibald G. Hill, Oklahoma State Univ
Adrian E. Johnson, Jr., Louisiana State Univ
Robert S. Kapner, The Cooper Union
Nazmul Karim, Colorado State Univ
Aydin Konuk, Oregon State Univ
Steven E. LeBlanc, Univ of Toledo
C. V. Metzler, California State Univ,
Northridge
Eugene Miller, Univ of Nevada, Reno
Robert D. Mohler, Ohio State Univ
Manfred Morari, Univ of Wisconsin
James O. Osburn, Univ of Iowa
Robert Pfeffer, City Univ of New York
J. Antonio Rocha, Univ of Texas, Austin
Robert P. Romig, San Jose State Univ
J. D. Seader, Univ of Utah
William J. Snyder, Bucknell Univ
William F. Stevens, Northwestern Univ
A. George Stoll, Cal Poly, Pomona
Spyros A. Svoronos, Univ of Florida
Amyn S. Teja, Georgia Tech
Normand Therien, Univ of Sherbrooke,
Quebec
Richard E. Thompson, Univ of Tulsa
Jim L. Turpin, Univ of Arkansas
Robert S. Weber, Univ of Delaware
Ronald D. Weir, Royal Military College of
Canada, Kingston
Reginald K. Wood, Univ of Alberta, Edmonton

**BATCH COMPUTING USING AN
ASYNCHRONOUS-TO-BISYNCHRONOUS
LINK BETWEEN A PERSONAL COMPUTER
AND A MAINFRAME COMPUTER**

by Professor Peter R. Rony

Remote job entry (RJE) stations and card readers are still used in many colleges and universities because of their low cost per student. Such stations are now being replaced by rooms of CRT terminals that are directly linked to the mainframe computer and available on a first-come, first-serve basis 24 hrs a day. This is as it should be because cards are obsolete in industry, and all engineering students should become facile with terminal-based computing. We have, however, observed a number of problems with the use of such time-shared terminals: a) computer science students are more tenacious than engineering students, who are not willing to sit in the hall for an hour and wait for a terminal; b) system response is not fast during editing sessions and slows considerably during the last week of a quarter (in other words, with more than 100 terminals on campus, our system is already overloaded); and c) terminal connect charges, which accrue every minute of terminal operation, become substantial when more than 100 undergraduate and graduate students are served in a chemical engineering department.

During the 1981-2 academic year, the Dept of Chemical Engineering at Virginia Polytechnic Institute & State University has been experimenting with an alternative to terminal-based computing. We have purchased a DATALYNX/3780 protocol convertor for RJE terminal emulation (cost, about \$1700) and have connected it directly to a Zenith/Heath Z89 personal computer, which has a CRT screen display of 80 characters by 24 lines that is perfectly suited for FORTRAN programming. We pay a monthly rental charge for a 9600 baud BISYNC line to the mainframe computer, but now enjoy the status of a full RJE station, which brings with it the following advantages:

- a) Priority - Our students now have higher priority than any of the other terminals on campus.
- b) Communication speed - Our students can now send programs and receive outputs at a communication rate of 9600 baud, in contrast to a rate of 2400 baud typical of terminals on campus.
- c) Low cost program compilation, execution, and communication - Fully edited programs are sent batchwise, and outputs are received

batchwise at the low cost typical of RJE station operation.

d) Off-line editing - Each Z89 personal computer has a single disk drive, and each student has his own disks that contain his own programs, the operating system (HDOS), the communications program (SUBMIT), and a screen-editor program (PIE80) that is as effective as is IBM 370 SCRIPT for writing FORTRAN programs.

e) Low-cost personal computer software - A license agreement is not required for the Zenith HDOS operating system, and copies can be made for each student. The PIE80 screen-editor software costs \$29.95 for the first computer, 50% of list price for computers 2 through 5, 20% of list price for computers 6 through 10, and 10% for each computer thereafter. We have seven Z89s in our computer room, so the total cost of running PIE80 on any Z89 computer by any student in the department is reasonable. We extensively modified a Heath User's Group communications program for our own use. Each student pays a very low one-time charge for one copy each of the software and the use of the computer room in the department. We use money to pay license fees for software.

No documentation is available on the chemical engineering RJE station so far, but you are welcome to visit the department and observe the system in use. An individual skilled in the setup and use of such a system would be available as a CACHE Consultant to another department of chemical engineering. For further details, please contact Dr. Rony.

PROGRAMS FOR MICROCOMPUTERS

Are you developing computer programs for microcomputers? If so, contact:

Professor Bruce A. Finlayson
Dept of Chemical Engineering
BF-10
University of Washington
Seattle, WA 98195

He is compiling a list of programs for microcomputers and identified at the ASEE Summer School several faculty members who are writing such programs. Bruce would like to know the subjects of your programs and the machine and operating system on which they operate.

**LIST OF INDUSTRIAL CONTRIBUTORS
TO CACHE**

The following companies contributed financial support to specific CACHE activities during the 1981-82 fiscal year:

Du Pont Committee on Educational Aid
Monsanto Fund, Monsanto Company
Shell Companies Foundation
The Halcon SD Group, Inc.

**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 1981-83 period as well as the just-concluded 1980-82 period are as follows. The latter departments are currently being solicited for the 1982-84 two-year period.

1981-1983

University of Alabama
Brigham Young University
Bucknell University
University of California, Davis
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
Univ 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

1980-1982

Arizona State University
Columbia University
University of Connecticut
Cornell University
Georgia Institute of Technology
Howard University
University of Idaho
University of Kansas
Kansas State University
Lafayette College
North Carolina State University
at Raleigh
University of Ntre Dame
Ohio State University
Princeton University
Rensselaer Polytechnic Institute
Rice University
Rutgers - The State University
San Jose State University
Texas A & I University
Tulane University
Villanova University
West Virginia Institute of Tech
McMaster University
Queen's University
University of Saskatchewan
University of Western Ontario
University of Windsor

MICROCACHE PROJECT

by Brice Carnahan

Abstract

The MicroCACHE (MicroComputer Aids for Chemical Engineering) Project involves the development of a microcomputer-based delivery system for educational materials and programs (educational "modules") for enhancing the quality and cost effectiveness of engineering education. The MicroCACHE Software includes a Supervisory System that processes MicroCACHE educational modules, maintains records of user progress, stores, and, in some cases, scores the results of examinations.

A MicroCACHE educational module consists of a sequence of screen displays, program executions, and interactions with the user (a student or practicing engineer) that might include display of textual information, display of graphical information, execution of engineering analysis, simulation and design programs, and administration of quizzes and examinations.

In its initial implementation, the MicroCACHE Project Software has been developed using an APPLE-II-plus microcomputer, equipped with a MicroSoft Z-80 Softcard.

Introduction Most engineering courses focus on information dissemination and the solution of single-answer, closed-end problems rather than the broader aspects of creative problem solving. A major reason for this emphasis is the lack of time available in the core courses to do more than teach the student to become proficient with engineering principles and to carry out fairly simple engineering calculations. The quality of engineering education can be enriched by allowing the student to spend more time on developing problem-solving capabilities with realistic problems and realistic data, while retaining the proficiency expected in engineering calculations.

A greater overall competence in design strategy and development of engineering intuition can be achieved by allowing students to generate and choose from a large number of alternative solutions. The advent of the personal computer makes possible the mechanization of many tedious calculations for the student working at home or the engineer working at the office. In addition to providing practice in the development of the student's synthesis skills, the personal computer can be used to execute interactive self-study programs of a tutorial or remedial

nature that will aid in obtaining better mastery of subject matter.

In order for students and faculty to capitalize fully on the revolutionary technological advances in personal computing, it is useful to develop, test, and evaluate models for rapidly infusing this technology into undergraduate education. The MicroCACHE (MicroComputer Aids for Chemical Engineering) Project Software is intended to demonstrate one such model for enhancing the quality of engineering education and enabling students (and practicing engineers) to profit from this personal computing capability.

The MicroCACHE Project involves the development of a microcomputer-based delivery system for educational materials and programs and the production of a small number of educational "modules" to test the system and demonstrate its effectiveness. The work is sponsored by the National Science Foundation and is being carried out at the University of Michigan.

Major Goals and Objectives We expect that the MicroCACHE System will serve as a model that will:

1. Improve the quality of education by providing the student (initially a chemical engineering student) with an interactive set of programs for personal computers which will help achieve greater mastery of the subject matter (initially, the subject matter of educational modules is chemical engineering; but in the future, any technical discipline could be the source of a MicroCACHE educational module).
2. Generate a greater degree of student enthusiasm for coursework by eliminating tedious, time-consuming calculations, particularly those of a repetitive or trial-and-error nature.
3. Allow for more cost-effective use of educational time by providing more time for developing problem-solving strategies and capabilities.
4. Allow faculty members to introduce more realistic examples and homework problems into courses as a consequence of the new computing capabilities of personal computers.
5. Encourage greater use of the new computational capabilities because a personal computer is accessible for use at a time and location of the student's own choosing.

6. Improve conceptualization (e.g., in data analysis) through graphical capabilities of new personal computers. This makes for a much more interesting, less tedious educational experience.

7. Allow for rapid distribution of portable programs and educational materials, thereby encouraging the infusion of this new technology (i.e., personal computers) into the educational process.

8. Provide the instructor with machine-readable information about individual student performance and progress and student evaluations of the programs and educational materials. With appropriate analysis programs, problem areas can be pinpointed; and the instructor can achieve student response and evaluation of educational materials on a one-to-one basis.

System Overview In its initial implementation, the MicroCACHE system is designed to operate on the APPLE-II-plus microcomputer equipped as follows:

- 1) 64K bytes of random access memory
- 2) two 5.25-inch minifloppy disks
- 3) the MicroSoft Z-80 Softcard
- 4) the MicroSoft Basic Compiler
- 5) a video monitor, either color or monochrome

To use the system, each user will need an educational module (MOD) diskette in conjunction with a personal MicroCACHE System Master (MSM) diskette. The System Master diskette contains the Supervisory System and is used to initialize the system, to control program execution, and to store certain kinds of information concerning the user (e.g., records of modules previously used). Each user will have a personal MSM diskette. An educational module occupies one diskette and consists of one or more submodules, such as lectures, exams, and calculation programs. Educational modules can be quite different in nature, and any module will operate in conjunction with the MSM diskette.

MicroCACHE Supervisory System The Supervisory System has the highest level of control over an educational module. It is responsible for loading and beginning execution of each module and, in most cases, supervising execution of submodules.

The user first invokes the Supervisory System by placing the MicroCACHE System Master diskette in the first disk drive of the APPLE (Drive A) and turning on the power. Thereafter the user can interrupt the execution of any module and return to the Supervisory System.

When the APPLE is first turned on, the Supervisory System begins by loading and displaying a title page. It then reads the access information found in the Module Command File (MCF), present on the module diskette. The MCF contains commands which are interpreted by the Supervisory System (functioning as an MCF command interpreter). The information contained on the MCF includes the title and number of the module, any access routes (lists of other modules required as prerequisites) which have been specified for the module, the number of times the module may be accessed, and a keyword index for the module. It then checks a file of user information stored on the MSM diskette to see if this module has been entered before. If access is allowed, the Supervisory System updates this file to indicate that this module has been entered, initializes any new files to indicate that this module has been entered, initializes any new files required, and displays a menu. The menu functions as a table of contents for the module, listing the various sections of the module which the student may select (each such section may consist of one or more of the MicroCACHE submodules).

Following the menu section of the MCF is a set of individual Supervisory System commands. These commands control the sequencing of the various displays, program executions, etc., as established by the module writer (e.g., a professor), and involve the display of text lines from "text files", text pictures from "graphics files," questions (possibly involving pictures) from "exam files," and "quiz files," execution of programs in "program files," and execution of programs from system "library files" (e.g., numerical analysis, graphics, and information storage/retrieval subsystems). The sequencing of Supervisory System commands can be quite rigid, or can be made conditional on user responses; the user can be given considerable flexibility in sequencing parts of the module (skipping over explanatory materials, deciding when to take an exam, etc.) if the module writer so chooses. A system program named "MODPREP" has been written to assist the module writer in preparing the MCF.

In addition to its principal function of processing module commands from the MCF, the Supervisory System is responsible for maintaining up-to-date records for each user, including, for example, which modules have been accessed and responses to examination questions (exams involving only multiple-choice questions or questions requiring numerical answers are automatically "scored," while those involving essay questions are not). Additionally, each module is terminated with an "evaluation" section, in

which the user can comment on the educational experience (pointing out errors or poorly constructed submodule sections, for example).

The MicroCACHE Supervisory System also includes an independent "analysis" subsystem for use by the instructor to process the information for a subclass of users (e.g., results of an examination for all members of a class or collective evaluations for a particular module).

General MCF (Module Command File) Commands

All Module Command File (MCF) commands consist of a one- or two-letter abbreviation immediately followed by a colon and then a parameter which is usually the name of a file on the MOD. Precise formatting of the commands is not required of the module writer since the Module Command File is prepared by the interactive MODPREP program. The MCF general commands follow in alphabetical order. With the command's syntactic prototype (items appearing in parentheses would be replaced by actual filenames, text, or labels in the MCF).

1) Branch Command:

This command is used to instruct the Supervisory System to branch to one of up to five labels following the colon in response to a number (1 to 5) entered at the keyboard by the student user.

2) Exam File Command:

This command is used to instruct the Supervisory System to load an examination file (named following the colon) from the MOD diskette and to begin presenting the user with an interactive examination. All exam files reside on the module diskette. Any answers collected by the Supervisory System are stored on the MSM diskette.

3) Graphics File Command:

GB: (graphics file name)

This command instructs the Supervisory System to load a binary graphics file from the MOD diskettes containing the exact image of a picture to be displayed on the monitor. These binary graphics files can be produced using the MicroCACHE Graphics Package, by software produced by the module writer directly. The APPLE II-plus uses 8K of memory (RAM) to define a high-resolution graphics page. This page is 280 columns by 160 rows (i.e., contains 44,800 pixels or positions where a dot can appear on the screen). By loading the graphics page with a picture and then saving it as a binary file, the module writer can prepare pictures for MicroCACHE modules. These pictures can be graphs, diagrams, equations, drawings, etc.

The menu section of the MCF contains up to 15 menu items which are displayed to the user. In the sample MCF, there are only three menu items. In addition to the three menu items that appear in the MCF, a fourth menu item is displayed to the user. This item (EXIT MICROCACHE SYSTEM) is used to exit the current MicroCACHE session.

Educational Modules Each educational module, when presented by the MicroCACHE Supervisory System Software, consists of displays and/or program executions as follows:

1. Screen displays of textual material
2. Screen displays of graphical (picture) material
3. Screen displays of question and/or examination material for which student response is expected.
4. Execution of programs appropriate to the module (for example, engineering design and simulation calculation programs).
5. An interactive module-evaluation session that concludes processing of the module.

These educational modules are designed to fit on one diskette. The student should be able to complete most modules in approximately one hour. The order of submodule presentation is determined primarily by the module writer (professor) and is controlled by the order of module "commands" prepared by the module writer and available to the MicroCACHE Supervisory System Software in the MCF. The module writer can allow as little or as much user (student) control over the sequencing as desired.

The latter is accomplished in two ways:

- 1) presentation of a menu from which the user can choose options and 2) use of a 5-way branch command in the MCF. The second can be employed to direct the MicroCACHE Supervisory System to take alternate paths through the MCF as a result of user responses to module-writer-initiated queries.

Three MicroCACHE system library programs have been prepared to help the module writer with the preparation of modules:

- 1) The graphics package: This general-purpose graphics program is available to assist in the preparation of graphs or line drawings in bitmap form suitable for storage in Graphics Files. The package can also be incorporated into calculation program files for generation of graphs or other drawings during execution of calculation programs.

2) The data-base management package: This is a general-purpose information storage and retrieval system that stores and retrieves labeled scalar or array data values in data files.

3) Numerical analysis package: This is a general-purpose set of routines for handling common numerical problems such

as solution of small systems of linear, nonlinear, and ordinary-differential equations, simple regression, numerical integration, etc. The routines are written in FORTRAN and available in object form for use as stand-alone programs. They also can be called from module calculation programs.

Lecture Submodules Lecture material is stored in a text file. The Supervisory System includes an interpreter capable of reading and displaying lines of text. The interpreter reads lines from the text file until a page is filled or it is told to stop, then pauses for a prompt from the user before starting a fresh page (either the next or immediately preceding page). Graphics pages can be displayed instead of text.

The text is logically broken up into sections for clarity. The user is always able both to page rapidly through the lecture material (a table of contents for the text files) and to exit back to the module menu. The principle is that the user need not wait or go through a procedure unnecessarily.

Exam and Question Submodules Test questions and answer choices are stored in a file in a manner analogous with the lecture material. Currently, all user responses to questions are input from the keyboard. In the future, user interaction from the game paddles and possible other input devices will be allowed.

Questions are generally phrased as a portion of a lecture. Two types of questions are available: multiple choice/numerical answer and essay answer. Thus the multiple choice question, "How many years until you graduate?" might appear to the user as follows:

- How many years until you graduate?
- A. None
 - B. Less than a year
 - C. A year or two
 - D. Too many
 - E. None of the above

Numerical answer questions include the question text, the correct numerical solution, and a tolerance (expressed as a percentage). The student is asked to enter an answer, and this answer is checked against

the correct answer (plus or minus the tolerance allowed). Multiple choice/numerical answer examinations are automatically scored by the MicroCACHE system.

Essay answer questions display only the questions. They may optionally include correct answers which are displayed after the user has responded to the question.

Exam submodules differ from question submodules in that the user's answers to examination questions are stored on the MSM diskette for later processing, while question submodule answers are not stored. As was mentioned previously, multiple-choice/numerical answer examinations are scored before they are stored on the MSM diskette.

Conclusion The MicroCACHE project has been underway since May of 1981. The overall system structure has been specified, and the module preparation and processing (Supervisory System) software has been written. We are now in the process of debugging the software and hope to begin testing the system with students in the fall of 1982. With results of the testing experience in hand, we will undoubtedly make changes in the system specifications and operation. Once the revised system is functioning reliably and a suitable distribution mechanism has been set up, the programs will be made available for use by others (probably in 1983). Those interested in obtaining further information should contact:

Professor Brice Carnahan
Dept of Chemical Engineering
Dow Bldg, North Campus
The University of Michigan
Ann Arbor, MI 48109

STATUS OF THE CHEMI PROJECT

by Professor David M. Himmelblau

The status of module preparation for the CHEMI Project is summarized as follows:

Status of New Module Preparation

Area	No. of Modules		
	to be Written	Commissioned	No. Completed (%)
Process Control	2	2	1 (50%)
Transport	25	10	4 (16%)
Material & Energy Balances	21	18	5 (24%)
Thermodynamics	22	16	3 (14%)
Kinetics	5	0	0 (0%)
Stagewise & Mass Transfer	12	2	2 (17%)
Design	20	27	10 (50%)
Advanced Level	70	26	6 (9%)
Total	177	101	31 (57%)

In addition, we have almost completed negotiating a license from the MIT Press to initiate electronic distribution of a number of the modules from Proceed Project. These modules are related to thermodynamic availability analysis, synthesis of heat exchanger networks, energy-saving opportunities, and the like. We are going to have to pay \$4,000 for the right to distribute these modules electronically but should obtain without difficulty approximately 30 of the so-called advanced modules that will be presumably well defined, well written, and in good style.

Work on the information system that is going to accompany the distribution of the modules is proceeding well. National Instruments, our subcontractor, has designed about 75% of the essential elements of the system, which is going to contain the following:

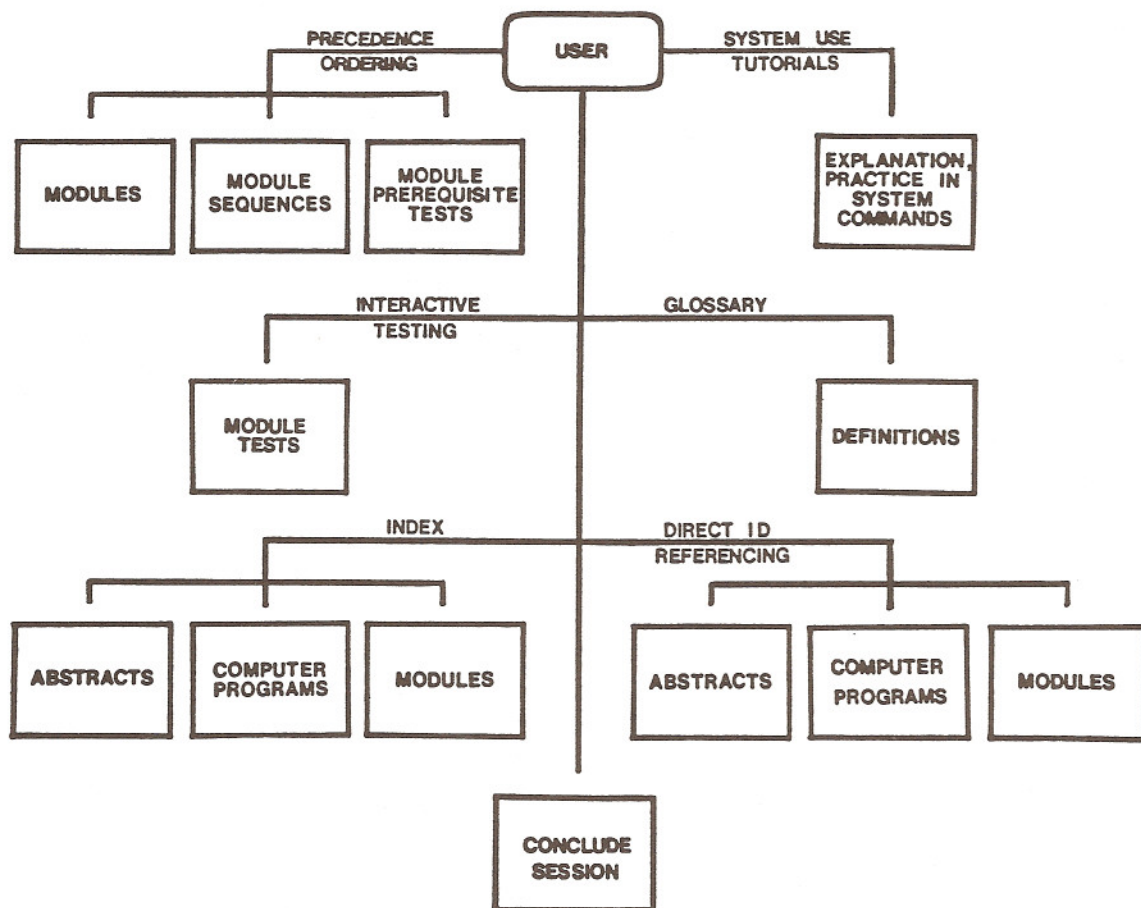
- 1) Data files in pre-specified format. Data files are files that will be displayed and printed.
- 2) Screens with menus. The screens will have on the left-hand side the possible choices for the user, and at the very bottom line the choice will be displayed. The balance of the screen will consist of instructions or abstracts or modules, whatever is currently being requested by the user.

A number of functions will be available to the user via the information system as shown

in the figure on the next page. Precedence ordering refers to the determination of paths from an initial module to the final module through a sequence of modules in the same series, or even a sequence from different series. The tutorials are merely advice to the user as to how to use the system in various ways. Interactive testing will probably not be implemented inasmuch as we do not have sufficient funds but would be an ideal function to add to the information system. We will have a glossary, an index, and methods of direct referencing to abstracts, computer programs, and modules. The user can, through the index, seek broader words, narrower words, similar words, prefixes, and so forth.

We are not having a complete system prepared inasmuch as we do not have funding for such a large-scale project. However, we are having the essential features of modules and abstract retrieval, key-word searching, precedence-order determination, and information about how to use the system prepared. We plan to code the information in Language C, which is currently the easiest language to use for the type of data base and information retrieval we will have and, in addition, is probably the only language that has fairly rigorous standards from machine-to-machine and operating system-to-operating system. C compilers are becoming available so that by the time the CHEMI Project materials are ready for distribution, we expect to find that various departments have the ability to run our software.

We have been testing various phases of the module entry into the computer and have paid particular attention to how the drawings and equations will be entered. It appears that we can put most of the material in a format that can be retrieved by a dumb terminal, but certain very complex figures will have to be issued as supplementary material to the tapes that we are going to distribute inasmuch as it is hopeless to enter such figures into our data base. In fact, even with the assistance of graphics terminals, a number of the figures would be far too complex to store and retrieve from a computer.



The CHEMI Project has about one year to run. However, it may be necessary to extend the life of the project at least six months to tie down all of the final details. Field testing will not be carried out until we have a good product.

GRAPHICS TASK FORCE NEWS

by G. V. Reklaitis

ASEE Summer School

The task force developed a program on computer graphics and modular instruction at the ASEE Summer School for ChE faculty held August 1-6 on the Santa Barbara campus of the University of California. Speakers included

Professors Michael Cutlip, Chuck Eckert, David Himmelblau, Rex Rekalitis, and Stanley Sandler. The evening lecture on CAD and Computer Graphics was given by Mike Bailey, the co-director of the CAD/Graphics Lab at Purdue University. The entertaining and informative lecture gave an overview of advances in 3-D and color graphics. Mike is a valuable resource person in graphics and may be contacted for advice in this area. To augment the lecture program, two hardware vendors, Tektronix and Megatek, participated with demonstrations of their graphics terminals on Monday and Tuesday afternoons. These companies, as well as CDC, who made available several PLATO terminals, are to be commended.

Graphics Superset

The task force is pursuing the possibility of developing a CACHE graphics software superset as well as a body of interfacing software to allow increased portability of applications software among academic users. Programs written using the superset conventions and command structure could be run with any vendor-supported graphics software package for which an interfacing software set has been developed. Individuals interested in contributing to this project are invited to contact the task force chairman.

Clearinghouse

The task force is continuing pursuit of funding for the establishment of a graphics software clearinghouse which would aid in the acquisition, distribution, and testing of software of chemical engineering orientation. Proposals have been submitted to both private foundations and governmental agencies with no positive response to date. Individuals interested in participating in pilot clearinghouse activities by contributing educationally oriented programs or by testing submitted programs at their site are invited to contact the Task Force Chairman, Professor Yaman Arkun of Rensselaer Polytechnic Institute.

TASK FORCE FOR THE DEVELOPMENT OF PROCESS DESIGN CASE STUDIES

by Manfred Morari

In addition to the announcement of the task force in the previous CACHE Newsletter, letters were sent to all chemical engineering departments in the country soliciting participation. About 20 positive responses were received, mostly from smaller schools, indicating varying degrees of commitment, prior involvement in case study projects, and industrial ties or experience. Some of the respondents provided problem statements of design projects. There was no industrial response. However, industrial participation might be possible through individual schools that teach design courses in cooperation with local companies.

Last semester a design project proposed by EXXON was completed independently by students at Carnegie-Mellon University and the University of Wisconsin with the goal of providing a sample case study to be provided as a guideline to participants. Though some excellent solutions were provided, they don't reflect the design process in all of its aspects; and significant modifications will be necessary.

The next steps to be taken by the task force will be:

- 1) Review committee consisting of James M. Douglas and Manfred Morari will work out a set of guidelines to preparing case studies.
- 2) Review committee will select three attractive and interesting project formulations and mail them to participants.
- 3) Interested participants agree to work on a project during spring semester 1983 together with students and hopefully industrial cooperation.
- 4) If a completed case study is found satisfactory by review committee (possibly after iterations), it will be issued by CACHE.
- 5) Task force meeting is planned during Los Angeles AIChE meeting in November, 1982.

PPDS (Physical Property Data Service)

With financial support from DuPont and Simulation Sciences, Inc., CACHE has leased, from the British Institution of Chemical Engineers, through the efforts of Professor Rudy L. Motard of Washington University, a version of the PPDS physical property retrieval and estimation program. The service is now installed on a DEC System 20 computer at Carnegie-Mellon University and can be accessed via the TELNET communication network, which provides local dial-up service in most cities.

Professor Motard has completed a user manual for PPDS entitled "Introduction to CACHE Version of Physical Property Data Service." Copies of the manual can be ordered by using the order blank at the end of this newsletter.

The CACHE version of PPDS provides retrieval of the 17 constant and 15 variable properties, in a variety of units, including S.I. and British, for 50 compounds.

Input to PPDS is interactive, wherein the user enters replies to questions from PPDS.

Output from PPDS consists of:

1. Tabulated, selected constant properties of pure compounds or mixtures.

2. Tabulated, selected variable properties of pure compounds or mixtures at specified intervals of T and P.
3. Warning messages for less reliable estimates.
4. Array values for user-written programs through FORTRAN interface.

In order to use CACHE-PPDS, contact:

Professor R. L. Motard
Department of Chemical Engineering
Washington University
St. Louis, MO 63130

He will send a contract and additional information. Upon receipt of the signed contract, a purchase order is sent to CACHE to cover an initiation fee of \$100 for CACHE-sponsoring departments or \$200 for non-sponsoring departments. This should be sent to:

CACHE
Room 3062 MEB
Salt Lake City, UT 84112

The approximate total cost to access CACHE-PPDS by TELENET is \$5 per connect hour, payable to Carnegie-Mellon University.

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

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 Michigan)

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
Manhaca, TX 78652

AICHEMI MODULAR INSTRUCTION SERIES AVAILABLE

AICHE has published six additional volumes of the AICHEMI Modular Instruction Series that 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. The 12 volumes now available are:

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CALL FOR PAPERS

One three-hour session (Session VIII) will be held for which contributed papers are hereby solicited on the topics covered by the invited papers session.

deadlines:

Extended Abstract: January 1, 1983
Manuscript: April 1, 1983

to:

Professor C. M. Crowe
Department of Chemical Engineering
McMaster University
Hamilton, Ontario L8S 4L7
CANADA

TOPICS:

Computer Science Aspects
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