CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 22

April 1986

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:

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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 aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by D.M. Himmelblau with contributions from a number of CACHE members and representatives.

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ANNOUNCEMENT

CONFERENCE ON FOUNDATIONS OF COMPUTER AIDED PROCESS OPERATIONS

The Computer and Systems Technology Division of AICHE (CAST) and CACHE plan to convene a specialist conference on the subject of process operations. This conference will focus on state-of-the-art research issues and needs, and will exclude tutorial materials more appropriate for a short course. The meeting will be held in July, 1987, in Park City, Utah and will be of one week duration. The meeting format will follow that of the highly successful FOCAPD (Design) and CPC (Chemical Process Control) conferences jointly sponsored by the two organizations, namely morning and evening technical sessions involving a few selected speakers and extended periods for discussion by the participants (See Table 1). Conference procedings will be published in hard cover form and will include transcriptions of key items of the discussions and summaries by the session chairmen.

The Conference Organizing Committee consists of the following academic and industrial members:

Rufus A. Baxley (Union Carbide)
Ignacio Grossmann (Carnegie-Mellon University)
John C. Hale (DuPont)
Richard S.H. Mah (Northwestern University)
F.A. Tony Perris (Air Products Ltd, UK)
Gary Powers (Carnegie-Mellon University)
Norman E. Rawson (IBM)
David W.T. Rippin (ETH, Zurich)
G.V. Rex Reklaitis (Purdue)
H. Dennis Spriggs (Linnhoff March)
George Stephanopoulos (MIT)

The conference co-chairs will be Reklaitis and Spriggs. Table 2 lists the session topics and chairmen.

Motivation for the Conference

It is now generally recognized that relatively few grass-roots chemical plants of world-class scale are likely to be designed and built in the USA and Europe in the next decade. Attention of the processing industry is instead being focused on the operation, improvement, and modification of existing plants, many of them of older design and of a multiproduct and/or batch nature.

The stimulii for the concerns with operational issues are numerous and include:

1. heightened international competition for traditional markets resulting in increased emphasis on product cost and quality;
2. the availability of low cost computer technology, communications networks, and electronic instrumentation;
3. rapid progress in new methodologies such as expert systems, robotics, database techniques, and sophisticated man-machine interfaces;
4. the well-publicized efforts towards automatization and computerized planning and operation in the discrete parts manufacturing industries.
5. recent international focus on safe operation of manufacturing facilities, especially those handling or processing hazardous materials.

However, in spite of the rising prominence of plant operations as a subject for discussion and management concern, computer aided plant operations have not yet been given the proper attention by the chemical engineering research community, either in industry or in academia. To be sure, workers in the process control and process design areas do on occasion address operations issues, but typically only in a fragmentary fashion. What is more, the academic training of chemical engineers continues to emphasize design at the almost total exclusion of operations. It is the purpose of this conference to redress this situation by providing a forum for an in-depth review of the problems and needs in this new area of chemical engineering research and application. We believe this conference will both stimulate research activity and encourage the introduction of operations issues in ChE academic programs.

The interrelated topics which form the overall area of computer aided plant operations and which must be considered in any study of the subject are many. They include the following:

process information gathering methodology and systems
quality monitoring and control
failure identification and recovery techniques
process safety and hazard analysis
reliability analysis
planning and scheduling of routine maintenance
maintenance of complex technology
scheduling of operations & resources
inventory planning and in-process storage allocation
plant retrofitting
integration of scheduling and control functions
movement of functions from off-line to on-line
on-line optimization
design of systems for operators rather than researchers

Because of the very broad range of issues which must be considered and methodologies which are relevant and applicable, we have chosen a matrix approach to the selection of conference topics. In the plan for this conference, we have focused both on the key problem areas which are central to plant operations as well as on the special uses that can be made in plant operations of generic methodologies whose applicability extends beyond operations. Thus, the session plan is divided into two principal parts: the first four sessions focus on problem areas (process data acquisition, safety, operations planning and maintenance planning) while the last four sessions address the specialized application of generic tools (simulation, optimization, computer technology, and expert systems) to operations. Table 3 summarizes the topic divisions.

The area of operations is particularly in need of strong collaboration between industry and universities. The subject needs the insights, problem perceptions, and priorities derived from industrial practice to be married to the analytic tools and interdisciplinary talents that can be brought to bear in the university environment to achieve rapid and meaningful progress. To enhance university/industry interaction, the conference plan projects a nearly equal balance between industrial and academic researchers in the composition of the organizing committee, the session chairs, session speakers, as well as the attendees.

Table 1
Model Session Format
(time in minutes)

(15)	Introduction/Overview (Session chairman)
(45)	Speaker #1
(45)	Speaker #2
(20)	Break
(15)	Commentator
(60)	Discussion
(10)	Summary of Issues (Session Chairman)

Table 2
Foundations of Computer Aided Process Operations
Proposed Topics & Session Chairmen

Sun Eve	Reception & Opening (Speaker)	Spriggs/Reklaitis
Mon-AM	Process Data Acquisition & Interfaces	John Hale (DuPont)
Mon-PM	Process Safety	Gary Powers (Carnegie-Mellon Univ)
Tue-AM	Operations Planning	David Rippin (ETH, Switzerland)
Tue-PM	Maintenance Planning	Tony Perris (Air Products, UK)
Wed-AM	Process Simulation	Rufus Baxley (Union Carbide)
Wed-PM	Process Optimization	Ignacio Grossmann (Carnegie-Mellon Univ)
Thu-AM	Plant Networks & Data bases	Norm Rawson (IBM)
Thu-PM	Banquet (Speaker)	Spriggs/Reklaitis
Fri-AM	Expert Systems in Operations	George Stephanopoulos (MIT)

Table 3
Scope of Selected Topical Sessions

Process Data Acquisition & Interfaces
- Interfaces to Processes and Laboratories
- Interfaces to People and Operations
- Data reconciliation and rectification

Process Safety
- Safety & Hazard Analysis
- Availability/Reliability Analysis
- (emphasis on off-line procedures)

Operations Planning
- Inventory management, materials requirements planning
- Production Scheduling methodology
- Operating Procedures: start-up, shut-down

Maintenance Planning
- Maintenance Information Systems
- Crew Scheduling
- Supplies & Spares Inventory Management
- CAD aspects of Maintenance

Process Simulation
- Role of steady state simulation: on-line models, off-line models use of flowsheeting systems
- Role of unsteady state simulation: plant scale dynamics and control; training simulators; start-up/shut-down

Process Optimization
- Structural optimization: plant retrofitting and modernization; highly contrained process synthesis
- Parameter optimization; multi-level plant optimization; energy management; on-line optimization

Plant Networks & Databases
- Data Management Systems
- Distributed Computer Architectures
- Information Networks

Expert Systems in Plant Operations
- Fault Detection
- Expert control
- Generation of Operating Procedures (emphasis on on-line procedures)

STATUS OF 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 would be made available on magnetic tape to departments of chemical engineering to install on their own in-house computers. Thus departments would be able to run FLOWTRAN on their own computers at no charge other than that of their own computer center. CACHE is continuing the supervision of the preparation of FLOWTRAN load modules for a wide variety of mainframe, supermini, and supermicro-type digital computers and the distribution of the modules on magnetic tape to those departments that order them. Instructional books on FLOWTRAN are already available through CACHE by using the order form at the end of this newsletter. FLOWTRAN tapes are now available for the following computers:

1. **DEC VAX 11-7XX** series of super minicomputers running with the VMS operating system.
2. **DEC 20XX** mainframe computer running with the FORTRAN-20, Version 7 compiler (9-track, 1600 BPI tape).
3. **UNIVAC 1100** series computers running under the EXEC 1100 (38R2/08) operating system with the FORTRAN 77-SID (1OR/A) compiler (9-track, 1600 BPI tape).
4. **Amdahl** computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).

5. **IBM** and IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and 43XX with the following operating system and FORTRAN compiler combinations:

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

6. **IBM PC-XT-370** personal computer operating in conjunction with an IBM mainframe.
7. **CDC Cyber** mainframe computers with the NOS operating system and a FORTRAN V compiler.
8. **Apollo Domain** work stations running with AEGIS operating system (program on floppy disks).
9. **Data General** MV super-minicomputers running with the AOS/VS operating system.

Conversions are also underway for the DEC 10, Honeywell, Sperry 90/80, DEC VAX under UNIX, and Prime machines. Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes but not for consulting. A total of 125 FLOWTRAN tapes and floppy disks have already been distributed to departments at the following universities for the computers indicated:

University	Computer	Operating System
University of Adelaide	DEC VAX 11-780	VMS
University of Akron	IBM 370/158	OS/MVS
Aristotle University of Thessaloniki	DEC VAX 11-730	VMS
Arizona State University	IBM 3081	OS1/MVS
Arizona State University	IBM 4341/G2	VM/CMS
Arizona State University	IBM PC-XT/370	DOS 2.0
University of Arizona	DEC VAX 11-750	VMS
Beijing Inst. of Chem. Technology	IBM 4341	VM/SP
University di Bologna	DEC VAX 11-780	VMS
Brigham Young University	DEC VAX 11-750	VMS
University of British Columbia	Amdahl 470	MTS
Brown University	DEC VAX 11-730	VMS
Bucknell University	Apollo DOMAIN	AEGIS
California State Poly. University, Pomona	CYBER 170-750	NOS 2.2
University of California Berkeley	IBM 3081/K32	CP/CMS
University of California Davis	DEC VAX 11-780	VMS
University of California San Diego	DEC VAX 11-780	VMS
Carnegie-Mellon University	DEC VAX 11-780	VMS
Case Western Reserve University	DEC 2060	TOPS-20
Christian Brothers College	DG MV/10000	AOS/VS
University of Cincinnati	DEC VAX 11-750	VMS
Clemson University	IBM 3081	MVS
Colorado Sch. of Mines	DEC VAX 11-750	VMS
Colorado State University	CDC CYBER 730	NOS 2.3
University of Colorado	DEC VAX 11-780	VMS
Columbia University	DEC 2060	TOPS-20
University of Connecticut	IBM 3081D	VM/CMS
(The) Cooper Union	DEC VAX 11-780	VMS
Cornell University	IBM 4341	VM/CMS
University of Delaware	DEC VAX 11-780	VMS
Drexel University	IBM 3081	OS1/MVS
Florida Institute of Tech.	DEC VAX 11-780	VMS
Florida State University	DEC VAX 11-750	VMS
Georgia Institute of Tech.	DEC VAX 11-750	VMS
Grove City College	DEC VAX 11-780	VMS
University of Houston	DEC VAX 11-780	VMS
Howard University	IBM 3033S	OS1/MVS
Illinois Institute of Tech.	DEC VAX 11-780	VMS
University of Illinois at Chicago	IBM 3081D	VM/CMS
Inst. Tecn. Est. Sup. de Monterrey	IBM 4381	VM/CMS
Iowa State University of Sci. & Tech.	DEC VAX 11-780	VMS
Iowa State University of Sci. & Tech.	NAS AS/6	OS/VS2 MVS
(The) Johns Hopkins University	DEC MocroVax II	VMS
Kansas State University	NAS 6630	OS1/MVS
Katholieke Universiteit Leuven	Amdahl 470/V8	VM/CMS
Kuwait University	UNIVAC 1100-62	EXEC
Laval University	DEC VAX 11-780	VMS
Lehigh University	CYBER 170-730	NOS 2.2
Louisiana State University	IBM 3081	VM/CMS
Louisiana Tech University	IBM 370	VM/CMS
University of Lowell	DEC VAX 11-780	VMS
University of Lowell	CYBER 170-825	NOS 2.3
University of Maine	IBM 3033, 4381	VM/CMS
Manhattan College	DEC VAX 11-780	VMS
University of Maribor	DEC VAX 11-750	VMS
University of Massachusetts	DEC VAX 11-780	VMS
University of Massachusetts	CYBER 830	NOS
McMaster University	DEC VAX 11-780	VMS
Michigan State University	Amdahl 5860	MTs
Michigan Techological University	UNIVAC 1100-80A	EXEC
University of Michigan	Amdahl 5860	MTS
University of Michigan	Apollo DOMAIN	AEGIS

University of Minnesota	Apollo DOMAIN	AEGIS
Mississippi State University	UNIVAC 1100-80A	EXEC
University of Missouri-Rolla	IBM 4381	MVS
University of Nebraska	DEC VAX 11-780	VMS
New Jersey Inst. of Tech.	DEC VAX 11-780	VMS
New Jersey Inst. of Tech.	Sperry 90/80-4	VS7
New Mexico State University	DEC VAX 11-780	VMS
University of New South Wales	DEC VAX 11-780	VMS
St. University of New York at Buffalo	DEC VAX 11-780	VMS
City College of City University of NY	DEC VAX 11-750	VMS
City College of City University of NY	IBM 4341	VM/CMS
(Brooklyn) Poly. Inst. New York	IBM 4341	VM/CMS
North Carolina State University at Raleigh	IBM 3081	VM/CMS
Northeastern University	DEC VAX 11-780	VMS
Northeastern University	DG MV/8000	AOS/VS
Northeastern University	DEC VAX 11-780	VMS
University of Norte Dame	Prime 850	Primos
Tech. University of Nova Scotia	DEC VAX 11-780	VMS
Oregon State University	CDC CYBER	NOS 2.2
University of Ottawa	Amdahl 470-A	VM/CMS
University of Pennsylvania	UNIVAC 1100	EXEC
University of Pennsylvania	DEC VAX 11-750	VMS
University of Pennsylvania	IBM 3081	VM/CMS
University de Pisa	IBM 3081	VM/CMS
Ecole Polytechnique-U. of Montreal	IBM 4341	VM/CMS
Pratt Institute	DEC VAX 11-780	VMS
University of Puerto Rico	IBM 4341	VM/CMS
Purdue University	CDC 6500	VSOS 2.1
Rensselaer Poly. Institute	IBM 3033	MTS
Rice University	DEC VAX 11-780	VMS
Rose-Hulman Institute of Technology	DEC VAX 11-780	VMS
Royal Military College of Canada	Honeywell DP39	CP6
Rutgers-The State University	NAS AS/9000	OS1/MVS
San Jose State University	IBM 4341	VM/CMS
University of Saskatchewan	DEC VAX 11-780	VMS
Universite de Sherbrooke	NAS 5000 E	OS/MVT
University of South Alabama	IBM 4341	CMS
South Dakota Sch., Mines & Tech.	CYBER 170-720	NOS 2.1
University of South Florida	DEC VAX 11-750	VMS
University of South western Louisiana	DEC VAX 11-750	VMS
Stevens Inst. of Technology	DEC VAX 11-780	VMS
Syracuse University	IBM 4341	VM/CMS
Texas Tech University	IBM 3033	OS1/MVS
University of Toledo	NAS 6650	VM/CMS
University of Toronto	DEC VAX 11-780	UNIX
Tuskegee Institute	DEC VAX 11-750	VMS
Universidad Nacional del Sur	DEC VAX 11-780	VMS
Universida de Concepcion	DEC VAX 11-780	VMS
University of Utah	UNIVAC 1100	EXEC
University of Utah	DEC MicroVAX II	VMS
Villanova University	DEC VAX 11-780	VMS
Washington University	DEC VAX 11-750	VMS
University of Washington	DEC VAX 11-750	VMS
University of Washington	CYBER 170-750	NOS 1.4
University of Washington	IBM 4381-P2	VM/CMS
Wayne State University	Amdahl V-8	MTS
West Virginia Inst. of Technology	Amdahl 470	VM/CMS
Widener University	DEC VAX 11-750	VMS
University of Wisconsin	UNIVAC 1100	EXEC
University of Wisconsin	DEC VAX 11-785	VMS
Worcester Polytechnic Institute	DEC 2060	TOPS-20
Yale University	IBM 3083	VM/SP

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

INTERACTIVE FLOWSHEETING PACKAGE FOR FLOWTRAN ON APOLLO WORKSTATIONS

Brice Carnahan
University of Michigan

Chris Jaeger, a chemical engineering Master's student at The University of Michigan working with me, has recently completed a general-purpose interactive graphical flowsheeting package for use on the Apollo Domain workstation network, and interfaced it to Monsanto's FLOWTRAN process simulator.

The package, called PFP (Process Flowsheeting Package) uses relational data structures for both graphical and process data, and set-theoretic operators for storage and retrieval operations. PFP uses the DIALOG package (Apollo software) for menu generation, and allows the user to draw the flowsheet interactively using menus and mouse (for unit selection, unit and stream placement, zoom operations, etc.). All input data (e.g., stream and equipment parameter values, simulator parameters, etc.) are entered interactively into forms displayed on the screen using keyboard and mouse.

The package generates a complete input file for FLOWTRAN, which is then processed (or can be edited) in the usual way. We are currently testing the program with a few students from our senior design class (using the FLOWTRAN load module prepared by Prof. Michael Hanyak at Bucknell, and distributed through CACHE), and plan to use the PFP/FLOWTRAN programs for all students in our design course in the Fall.

Once we've tested the program thoroughly with a full class of students in the fall, we will make it available to other ChE departments with access to Apollo workstations.

MICROCACHE VERSION 1.1 RELEASED

Brice Carnahan
University of Michigan

A new version (1.1) of the **MicroCACHE** Software for Computer-Assisted Instruction on IBM Personal (PC,XT,AT) and IBM-compatible Computers was released on March 1. Hardware requirements are 256 Kbytes of RAM, at least two (floppy and/or hard) disk drives, and a color-graphics adapter (with monocolor or color monitor); a printer and/or floating-point processor (Intel 8087 or 80287) are optional, but quite useful.

MicroCACHE consists of (a) system software for preparation and presentation of educational modules (lessons), and (b) several already-written modules covering some topics in chemical engineering and numerical mathematics. The menu-driven presentation software:

1. Controls student access to modules (via passwords, module path specifications).
2. Presents screen displays of text and graphics, allowing for easy jumping from frame-to-frame to find desired information (selection based on Tables of Contents).
3. Executes calculation programs.
4. Administers examinations consisting of multiple-choice (MC), numerical response (NR), and essay questions (it scores MC and NR questions if desired).
5. Allows for on-line user evaluation of the materials.
6. Automatically maintains user records, including examination responses and scores and evaluation responses, and generates user data files.

MicroCACHE runs under PC or MS DOS (Versions 2.0 or later). Normally, MicroCACHE is run in a two-disk configuration. The supervisory software and user data are stored on the MSM (MicroCACHE System Master) diskette inserted into Drive A: and module related files are stored on the MOD diskette (Drive B:) or MOD hard disk subdirectory (Drive C:). However, MicroCACHE can be installed on virtually any IBM PC machine configuration (with up to six drives) including Local Area Networks with DOS-compatible operating systems. For example, we have successfully installed MicroCACHE on a 3Com Ethernet LAN with three 3Com file servers and 60 IBM PCs, XTs, and ATs, and administered quizzes to 550 students in a freshman computing course with all information retrieved from and stored on the LAN servers.

MicroCACHE module sequencing is controlled at first level by user menu choices. For each menu choice, the module writer controls submodule sequencing by a MicroCACHE "subprogram" consisting of simple MicroCACHE commands ("Display text", Run a program", "Administer an exam", conditional "Branch", etc.).

Several programs are supplied to help module writers prepare new modules. The most important are:

(a) TEXTPREP	Prepares screen frames from "unprepared" ASCII text files.
(b) EXAMPREP	Prepares quizzes and examinations from "unprepared" ASCII files containing questions and answers.
(c) MODPREP	Prepares the Module command file (creates menus, controls module sequencing).
(d) GRAPHICS	BASIC and FORTRAN graphics packages for preparing static graphic screens or generating dynamic graphics displays (usually for results in calculation programs.)
(e) RETRIEVE	Retrieves user-generated information stored by the MicroCACHE supervisor.

Virtually any executable file can be run as a calculation program. Typically, these are assembled or compiled programs present in (.EXE or .COM) DOS program files. We have used compiled (IBM) BASIC and Microsoft FORTRAN-77 programs for our modules, but other language compiler (e.g., C, PASCAL) can also be used.

The major new features incorporated into Version 1.1 are:

(a) Interpreted BASIC programs can now be run as calculation programs. The full features of the BASICA interpreter are available, and the BASIC programs are executed under MicroCACHE control with no reduction in execution time. The only restriction is that the SYSTEM command must be the logically last statement to be executed by BASICA.

The BASICA interpreter must be copied onto the module diskette (PC) or be available in some subdirectory (any one will do) on the hard disk (XT and AT). This feature should prove very useful for the documentation and presentation of BASIC programs being developed under auspices of the Curriculum Task Force.

(b) The module-writer can "Run" prepared DOS Batch (.BAT) files as well as calculation program files (or can create and then run batch files during presentation of a module).

The software is documented in six parts:

Introduction
System Overview
User's Manual
Instructor's Manual
Module Writer's Manual
Graphic's Packages User's Manual

The documentation (including two video-tapes), the system preparation and presentation software, and one module (for binary distillation by the McCabe-Thiele method) is available through CACHE for a cost of $400 per department. Several additional chemical engineering modules (interactive graphical process flowsheeting, steady-state simulator for solving material balances in recycle systems, Ponchon Savarit method for binary distillation, batch binary distillation, and gas reservoir simulation) are available, typically for $90. each per department. We also have or are developing several modules for solving numerical, optimization, and statistical problems as well. The complete list is shown on the order form at the end of this newsletter.

If you are interested in seeing a copy of the *System Overview Document* (29 pages), or would like to have a one-page description of the contents of any of the available modules, write to:

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

The software is copyrighted, but not copy protected. Permission is given to a purchasing department to make as many copies of the module preparation software as there are departmental faculty, as many copies of the module presentation software as there are departmental students, and as many copies of the module software as there are departmental machines. Permission is also granted to reproduce the written documentation as required to meet departmental needs. Each department (whether ChE or not) is required to purchase its own copy of the MicroCACHE software and documentation.

As of mid-March, we have shipped MicroCACHE software to 17 chemical engineering departments. We hope that MicroCACHE will be used in these and many other departments, and that faculty will begin to create their own modules this summer, and will be willing to share them with others through CACHE. The MicroCACHE Task force will handle distribution of information about MicroCACHE and module development through a Newsletter.

TASK FORCE FOR THE DEVELOPMENT OF PROCESS DESIGN CASE STUDIES

Manfred Morari, California Institute of Technology
and
Ignacio Grossmann, Carnegie-Mellon University

The CACHE Task Force on Process Design Case Studies under the direction of Professors Manfred Morari and Ignacio Grossmann has completed several activities. The two following new design case studies are now available:

Case Study 2. "Design of an Ammonia Synthesis Plant"

Case Study 3. "Preliminary Design of an Ethanol Dehydrogenation Plant"

These case studies make use of the simulators PROCESS and the CACHE version of FLOWTRAN, and they also include listings of programs for the simulation of chemical reactors. Both case studies emphasize the systematic synthesis of the process flowsheets. The two case studies can be ordered from Professor Brice Carnahan at the University of Michigan. The order forms and summaries of these case studies can be found in the last pages of this Newsletter. For each case study the price for the first copy is $15 for departments who currently provide financial support to CACHE. The price is $35 for additional copies, as well as for departments that currently do not support CACHE.

Professor Michael Malone from the University of Massachusetts is currently preparing a case study that deals with the design of a styrene process from methanol and toluene. This project is based on the 1985 AIChE Student Contest Problem, and it emphasizes the use of preliminary screening techniques. This case study should be completed in the summer.

The problem statement of a new case study is also available. The project deals with the design of a batch facility for manufacturing an animal grade antibiotic. The problem was prepared by Mr. Stuart Bacher from Merck Co. and by Professors Arthur Westerberg and Michael Domach from Carnegie-Mellon University. Data for the economic evaluation and for the manufacturing recipe are included. This problem emphasizes the design and scheduling of batch processes. The statement of this problem and of other design projects can be requested from:

Manfred Morari
Chemical Engineering, 206-41
California Institute of Technology
Pasadena, CA 91125
Tel: (818) 356-4186

or

Ignacio Grossmann
Department of Chemical Engineering
Carnegie-Mellon University
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Tel: (412) 268-2228

We would like to encourage faculty who teach design to submit reports for their possible publication by CACHE. Design case studies of particular interest are projects that deal with nonconventional technologies (e.g. biotechnology, electronic materials), or that illustrate the use of novel design and computing techniques.

ANNOUNCEMENT OF AVAILABILITY OF COMPUTER CODES

MICRO-DSS
For Ordinary and Partial Differential Equations with Color Graphics

Micro-DSS, a micro (personal) computer version of DSS/2, is now available for the numerical integration of systems of initial-value ordinary differential equations (ODEs) and one and two-dimensional partial differential equations (PDEs). Color graphics are included with Micro-DSS for displaying the solution to the ODE/PDE problem system.

Currently, Micro-DSS can accommodate:

(1) Up to 250 initial-value ODEs. All ODE integrators have automatic step size adjustment for error monitoring and control.

(2) One and two-dimensional parabolic PDEs, e.g., the heat conduction equation, with fourth-order (five-point centered) approximations of the spatial derivatives.

(3) As special cases of (2), two-point boundary value ODEs and elliptic PDEs through the method of false transients.

(4) One-dimensional hyperbolic PDEs, e.g., convective and convective-diffusion equations, with fourth-order (five-point biased upwind) approximations of the spatial derivatives.

A specific hardware/software configuration has been selected for the initial release of Micro-DSS:

IBM AT with 512Kb memory
IBM (Ryan-McFarland) Professional Fortran
Color or enhanced graphics adapter and monitor

A demonstration disk and a set of five manuals are available for evaluation of Micro-DSS. The demonstration disk contains software for significant problem solving (up to 250 initial-value ODEs with plotting of the solution in color).

Prices for the demonstration disk, and single-machine and site-license copies are available from: W.E. Schiesser, Whitaker No. 5, Lehigh University, Bethlehem, PA 18015 USA.

DSS/2
DIFFERENTIAL SYSTEMS SIMULATOR, VERSION 2
SINGLE AND DOUBLE PRECISION

DSS/2 is a library of transportable, Fortran subroutines for the numerical integration of systems of initial-value ordinary and partial differential equations (ODE/PDEs) with broad application in the computer analysis of large-scale systems in science and engineering.

DSS/2 can accommodate PDEs in one, two and three spatial dimensions in any regular orthogonal coordinate system, e.g., Cartesian, cylindrical or spherical coordinates. The ODE/PDE system may be linear or nonlinear.

The Fortran 77 source code is now available in single and double precision and can therefore be used on computers with word lengths ranging from 32 bits, e.g., IBM 30XX mainframes and DEC VAX, to 64 bits, e.g., CDC Cyber, CRAY and IBM 205.

The following manuals are available for Release 3:

Manual 1
Introductory Programming Manual (for ODEs)

Manual 2
An Introduction to the Numerical Method of Lines Integration of Partial Differential Equations

Manual 3
Numerical Method of Lines Integration of Partial Differential Equations in Cylindrical and Spherical Coordinates

Manual 4
Numerical Method of Lines Integration of Partial Differential Equations in Two Dimensions

Manual 5
Numerical Method of Lines Integration of First-order Hyperbolic (Convective) Partial Differential Equations

Manual 6
Variable-grid Spatial Differentiators in the Numerical Method of Lines

Manual 7
Numerical Method of Lines Integration of Partial Differential Equations in Three Dimensions

Also, some 150 applications running under DSS/2 in separations, kinetics and reactors, heat transfer, fluid flow and process control are available. Each application is a set of documented Fortran subroutines called by DSS/2.

The Fortran 77 source code is available on nine-track tape, along with a listing of the tape identifying the major sections of the code, the set of seven manuals and the output from ten test problems; all of the problems in the manuals and the test problems are included on the tape.

Inquiries concerning DSS/2 should be directed to:

Dr. W.E. Schiesser
Whitaker No. 5
Lehigh University
Bethlehem, PA 18015 USA

ODEPACK

A set of Fortran subroutines for the numerical solution of algebraic and initial-value ordinary differential equations.

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

(1) LSODE (Livermore Solver for Ordinary Differential Equations)

The basic solver for systems of ODEs, i.e., dy/dt = f(t,y), with full or banded processing of the Jacobian matrix of f(t,y).

(2) LSODI

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

(3) LSODA

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

(4) LSODAR

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

(5) LSODES

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

(6) LSOIBT

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

All of the integrators have nonstiff options (based on Adams formulas) and stiff options (based on BDF formulas). They are written entirely in transportable Fortran in single and double precision format. Each includes a demonstration problem, and a user's manual, provided as an extensive set of comments at the beginning of each integrator.

Arrangements have been made with Dr. Hindmarsh to distribute ODEPACK on nine-track tape for a nominal preparation charge. Direct requests to W.E. Schiesser, Whitaker No. 5, Lehigh University, Bethlehem, PA 18015 USA. The charge, which includes the tape, is $50.00 in the USA and $75.00 to other countries. Shipment is by U.S. Priority Mail or international air mail. Prepayment should be made as a check, payable to Lehigh University.

The tape format will be nine-track, 1600 bpi, ASCII, unlabeled, 80-character records, 10 records/block, unless otherwise specified.

LARGE SCALE SYSTEMS
Jeff Siirola
Eastman Kodak Company

As first reported in the last issue of CACHE News, the Large Scale Systems Task Force is currently working in two main areas including the development of an optimization capability enhancement for the CACHE FLOWTRAN process simulation program, and the search for additional computer-aided systems design tools suitable for use by the educational community.

The search for appropriate programs has been broadened to include several alternatives for steady-state and dynamic simulation as well as process synthesis. Suitability testing has begun on some routines and licensing negotiations are nearing completion to obtain the rights to test others. Testing and evaluation will continue throughout the Spring and Summer to be followed by the preparation of necessary documentation. If all goes well, the first of these programs will be ready for distribution in the Fall.

The FLOWTRAN optimization capability has been expanded by Professor L.T. Biegler to include several variants of the "feasible path" method in addition to the original "infeasible path" approach. The development of the algorithms and of their interfaces with the FLOWTRAN system has been completed and is now being tested at a number of universities. Documentation preparation is also underway for inclusion in the next edition of the FLOWTRAN manual. At this time, plans call for distribution beginning in late Summer. Specific details will be announced later.

PROGRAM PROFIT

Program PROFIT is available from Bruce Finlayson at the University of Washington, Department of Chemical Engineering, BF-10, Seattle, WA 98195. This program for the Macintosh does a discounted cash flow analysis of an investment or a series of investments. The information such as capital investment, revenue or expenses, can be different each year or the same from year to year. The user must define the investments by specifying the capital investment, when it is made, when the service life begins and ends, what the working capital is and the salvage value. The revenue and expenses are also specified year by year. The tax rate is specified, and the method of depreciation is either straight-line, double-declining balance, or sum-of-years digits. The program then calculates the discounted cash flow rate of return.

Use is made of pull-down menus with convenient data entry procedures. For example, data fills automatically from year to year so that the data entry is easy, although the automatically-chosen parameters can easily be selected and changed by the user. The program has a glossary giving definitions of terms and tells how they are used in the program.

Availability: Version 1 has been used in class and is available now. To receive a copy you need to send a Macintosh diskette to Professor Finlayson along with a statement agreeing not to copy the PROFIT diskette you receive. This unfortunate restriction is due to the restrictions Microsoft places on its BASIC runtime interpreter. [You can send as many diskettes as you like, however. Professor Finlayson has a license to duplicate them. If you buy Microsoft's runtime interpreter ($250) you can duplicate them.]

Version 2 will be compiled and will have no such restrictions. It will also plot the discounted cash flow versus time, and will allow both calculations and plots for different, specified interest rates. The date of availability is uncertain and will depend on when BASIC compilers are available in the marketplace (they've been promised by a least one company by March, 1986).

THE CACHE NATIONAL ELECTRONIC MAIL EXPERIMENT: PART 1. COMPMAIL +

by Peter R. Rony, John C. Hale, and Joseph D. Wright

INTRODUCTION

To quote the April 9, 1985 CACHE Electronic Mail Task Force proposal [1]: "The objectives of the CACHE National Electronic Mail Experiment are: (1) To catalyze the creation of a widely used national chemical engineering electronic mail network between academic, industrial, and government sites. (2) To issue a report that documents concrete examples of how to use electronic mail, identifies potential chemical engineering applications, and lists typical costs. (3) To extend such a network to our international colleagues. (4) To publicize the use of electronic mail in CACHE, CAST, AIChE, and other chemical engineering organizations. (5) To identify important uses for electronic mail in chemical engineering. (6) To perform limited tests of alternative electronic mail services. (7) To publish an article on electronic mail in CEP. (8) To generate goodwill for CACHE.

Publicity for the CACHE National Electronic Mail Experiment appeared in/at: (a) CACHE News, September 1984; (b) CAST Communications, April 1985; (c) CACHE Reception, 1984 National AIChE Meeting, San Francisco, November 1984; (d) "The IEEE Electronic Mail System," a presentation by Peter Rony at the 1985 Spring National AIChE Meeting, March 1985; (e) a memorandum sent by CACHE to member chemical engineering departments, August 1985; and (f) CACHE Reception, 1985 National AIChE Meeting, Chicago, November 1985.

The timetable for expansion of the CACHE National Electronic Mail Network was proposed to be [1]:

April 1985	40-50 mailboxes	(all CACHE sponsored)
Nov. 1985	50-100 mailboxes	(50 CACHE sponsored)
April 1986	100-150 mailboxes	(50 CACHE sponsored)

Members of the chemical engineering community were invited to participate in a CACHE National Electronic mail experiment based upon a commercial electronic mail service, COMPMAIL+, that is widely used by officers, staff, and members of the IEEE Computer Society; the American Bar Association; the White House News Service; and other organizations. Few colleagues did so other than members of the CACHE Board of Trustees and 1985 CAST Executive Committee, each of whom was automatically given both a COMPMAIL+ account and instructions how to use it. As of January 31, 1986, CACHE sponsored 55 COMPMAIL+ mailboxes, 35 of which were never used; five mailboxes were financed privately. The installation of these mailboxes was completed by April 30, 1985.

$1200 was requested to defray the expenses of the first partial year (November 21, 1984 to June 30, 1985) of the CACHE National Electronic Mail experiment [1]; an additional $2000 was allocated for the period, July 1, 1985 through June 30, 1986. Between November 1984 and December 1985, a total of $1724.04 was spent. Monthly charges--and, of course, monthly usage--steadily declined from a peak of $262.40 during June 1985 to $105.00 during December 1985.

DEMONSTRATED USES FOR COMPMAIL +

The use of COMPMAIL+ to transfer files for CAST Communications accounted for perhaps $30-$40 per newsletter worth of charges during March 1985 and August/-September 1985. About twenty, single-spaced, typeset pages of text were sent each time, for a cost of "saving keystrokes" of about $2 per page. The value of the time spent by Peter Rony in entering the text into a personal computer, and by Joe Wright and Debbie McPhail in editing, formatting, and printing the newsletters, far exceeded the costs of electronic mail communication. Article files were also sent to David Himmelblau at the University of Texas for publication in CACHE News. These are two examples where COMPMAIL+ can improve productivity and be cost effective.

As reported in the August 10, 1985 memo to chemical engineering departments [2], the use of electronic mail included the transmission of files for publication in a newsletter, iteration of manuscripts for publication, transmission of messages among CAST officers and CACHE trustees, planning the registration for a conference, and iteration of several chapters in a PhD thesis. Despite the invitation by and willingness of CACHE to fund costs for several months on an experimental basis, little interest in participating in the experiment was exhibited by other faculty members in the chemical engineering community.

An attempt was made to create a CACHE chemical engineering bulletin board associated with COMPMAIL+. This attempt failed, since it was not possible to create sub- or multiple bulletin boards; the IEEE COMPUTER SOCIETY had its own COMPMAIL+ bulletin board, and no other was possible.

CONCLUSIONS

The first phase of the CACHE National Electronic Mail experiment has not been a rousing success; a small step for chemical engineering wide-area networking and a learning experience...but nothing more.

The addition of CACHE-funded COMPMAIL+ accounts will not cease, and all accounts that are not being used will be closed. By April 1986, there should be no more than 10-15 accounts, most of which will be active. Even these accounts will be phased out when an alternative wide-area network for the chemical engineering community becomes successful.

The human interface--the need for a new user to assemble the necessary computer and communications hardware and software, select an electronic mail network, learn new commands and procedures, and perhaps obtain computer funding--presents an unfortunate and serious barrier, for busy professionals, to the spread of electronic mail within the chemical engineering community.

Despite publicity--at AIChE meetings, through CACHE News and CAST Communications, and through a CACHE mailing to chemical engineering departments--interest in electronic mail remains low in the chemical engineering community. We, along with some of our sister engineering disciplines, lag behind other disciplines in incorporating electronic mail as an active and vital communications link between professionals. For example, and with no surprise, most academic computer scientists actively participate in electronic mail communications through their self-financed network, called CSNET.

CACHE can play a catalytic role by identifying acceptable electronic mail networks and disseminating information on how to gain access to them. A particularly desirable result from experiments conducted by the CACHE Electronic Mail Task Force would be an ability to use electronic mail to rapidly communicate with colleagues overseas. CACHE is in no financial position to fund electronic mail beyond our one-year experiment that demonstrates the value of this form of communication.

An important objective that remains for the CACHE Electronic Mail Task Force is the identification of the electronic mail service that is most cost effective on a long-term basis for chemical engineering departments. The next phase of the CACHE National Electronic Mail experiment will focus on a more popular academic wide-area network, BITNET. BITNET may be the preferred network for universities, both domestic and foreign, because of its low or zero cost to chemical engineering department (only "funny money" is needed on many campuses).

The national Science Foundation is exploring the logistics associated with creating and maintaining a national electronic mail capability, called NSFnet, for all science and engineering professionals in the United States. It is important that the AIChE monitor such development. For preliminary details, consult the recent article, "Computer Networking for Scientists" in the February 28, 1986 issue of Science.

An open-access network is essential for electronic mail communication among chemical engineering colleagues in academia, industry, government, and at AIChE headquarters.

Among a group of 50 active professionals in the computer area, a reasonable percentage, approximately 25%, became users of electronic mail during the CACHE National Electronic Mail experiment with COMPMAIL+. Approximately 10% of these 50 professionals became very active users.

Costs for the COMPMAIL+ experiment were held to reasonable levels, but could have exploded in as little as one month if, for example, 50 supported users each consumed $10 per person in electronic mail services. COMPMAIL+ communications by Telenet or Tymnet occasionally proved to be troublesome because of overloaded networks or line noise; such problems frustrate electronic mail users and make the error-free transmission of information much more difficult.

REFERENCES

1. Peter Rony, "The CACHE National Electronic Mail Experiment," CACHE Communications Task Force Proposal, April 9, 1985.

2. Peter Rony and John Hale, "Fall 1985 CACHE Electronic Mail Experiment," Memorandum sent to chemical engineering departments, August 10, 1985.

THE CACHE NATIONAL ELECTRONIC MAIL EXPERIMENT: PART 2. BITNET, ARPANET, AND NSFNET

by Peter R. Rony, Chairman, CACHE Electronic Mail Task Force

INTRODUCTION: COMPUTER NETWORKING FOR SCIENTISTS

The article, "Computer Networking for Scientists," which was published in the February 28, 1986 issue of *Science*, is recommended reading for all chemical engineering faculty who are interested in wide-area networking. It is an early public source of information on NSFnet, which "will probably have the most impact on science of all networking activities in the United States at this time." The article discusses plans for NSFnet, and includes a "List of planned member institutions" (glance at Table 2 in the article to see if your institution is on the initial list; mine is not).

The deadline for the spring issue of CACHE News was February 28, 1986, and this article is a last-minute contribution. The CACHE Electronic Mail Task Force has not had time to request permission of the publishers of *Science* to reprint the above article so that it could be sent to member departments of CACHE for circulation among their faculty. We would appreciate it if departments would assume this responsibility.

Briefly, the *Science* article discusses NSFnet and then outlines the history and characteristics of the following major scientific, engineering, academic, government, and military wide-area networks in the United States:

ARPANET
CSNET
BITNET
MFENET
UUUCP
USENET

Other wide-area networks--SPAN, NAS network, the planned high-energy physics network--are mentioned but not discussed. The article concludes with a brief survey of state networks--for example, the Merit Computer Network in Michigan, NYSERNet in New York, the Princeton consortium network, the San Diego consortium network, the supercomputer "backbone" network--and campus networks. Several CACHE trustees have had two years of experience with the Michigan Merit Computer Network.

Interesting points made in the *Science* article include the following:

"The major lesson from the ARPANET experience is that information sharing is a key benefit of computer networking. Indeed it may be argued that many major advances in computer systems and artificial intelligence are the direct result of the enhanced collaboration made possible by ARPANET."

"However, ARPANET also had the negative effect of creating a have-have not situation in experimental computer research. Scientists and engineers carrying out such research at institutions other than the twenty or so ARPANET sites were at a clear disadvantage in accessing pertinent technical information and in attracting faculty and students."

"In the beginning, the need for CSNET was not universally accepted within the computer science community. However, the momentum created by CSNET's initial success caused the broad community support it now enjoys. More than 165 university, industrial, and government computer research groups now belong to CSNET."

"Although initially designed for supercomputer users to gain access to supercomputers and to communicate with each other, NSFnet is expected to be a general-purpose computer communications network for the whole academic research community and associated industrial researchers."

"The general strategy recommended by the networking panel report was that the NSFnet should begin by taking advantage of the existing academic networks. NSFnet should be built as a 'network of networks' rather than as a separate new computer network."

"A common set of networking protocol standards has, therefore, to be adopted by NSF in order to build the NSFnet Internet. NSF has decided on the ARPANET protocol (TCP-IP and associated application protocol--the DARPA protocol suite) as the initial NSFnet standards."

"By September 1986, on the basis of the developments planned to date and of the expansion of the ARPANET, more than 60 major research universities in the United States are expected to be connected to NSFnet, to the NSF supercomputers, and to each other (Table 2). Other institutions are expected to be added to this list during 1986."

"Most BITNET sites use the same electronic mail procedures and standards as the ARPANET, and as a result of the installation of electronic mail gateway systems at the University of California at Berkeley and at the University of Wisconsin--Madison, most BITNET users can communicate electronically with users on CSNET and the ARPANET."

"The average researcher working at a terminal or workstation at one of these institutions will then be able to connect to and use various computer resources--including the NSF supercomputer centers--to run interactive and batch jobs, receive output, transfer files, and use the electronic mail facilities to communicate with any colleague throughout the nation. Typically, an individual research will have either a terminal connected to a local super-minicomputer or a graphics workstation. These computers will be connected to a local area network (LAN) that will provide local communications and resource sharing. It is expected that this LAN will itself be connected to other LAN's on the campus, and that the collection of interconnected LAN's will form a campus network--with, ideally, a campus-wide service organization taking responsibility for the overall network services provided. In turn, this campus network will be connected, via a campus gateway system, to one or more of the wide-area networks in the NSFnet to provide the research with computer communications across the United States."

WIDE-AREA NETWORKING IN CHEMICAL ENGINEERING

In the light of the announcement of plans for NSFnet, how should the chemical engineering community respond? As a start, I recommend that individual chemical engineering departments take the following steps:

1. Scan Table 2 in the Science article, "Computer Networking for Scientists" [Science 231, 943-950 (28 February 1986] to determine if your college or university is included

on the list of planned member institutions. If not, contact your campus-wide computer service organization and inquire about inclusion in NSFnet.

2. Poll departmental faculty to determine who is on ARPNET, BITNET, CSNET, or any other wide-area network. Obtain userids for faculty members who wish to use electronic communication in the near future. Submit a departmental list of names and userids to Peter R. Rony (Department of Chemical Engineering, Virginia Tech, Blacksburg, Virginia 24061) for publication in a forthcoming CACHE listing of wide-area network userids for chemical engineering.

3. Commission an interested undergraduate or graduate student in your department to (a) test and simplify the documentation of procedures for accessing BITNET and ARPANET, and (b) assist faculty to make use of such networking services.

4. Submit information on existing departmental uses of wide-area networking to me, John Hale, or Joseph Wright (CACHE Trustees who are members of the CACHE Communications Task Force) for condensation and publication in future issues of CACHE News. Identify an interested faculty member who would serve as the contact person between the department and the CACHE Electronic Mail Task Force; send his name to me.

5. If you seek information about the growing list of BITNET chemical engineering userids and their respective university nodes, please contact me at any time. My university phone number is (703) 961-7658.

INITIAL LIST OF BITNET USERIDS

In response to an August 10, 1985 memorandum to chemical engineering departments, as well as inquiries at the Chicago National AIChE meeting, the following colleagues either already have BITNET userids or else are interested in becoming a contact person for information about BITNET.

Tom Wayburn (USEREUOO at CLUM), Clarkson University
John C. Hassler (RCG360 at MAINE), University of Maine
Raul Miranda (ROMIRA01 at ULKYVM), University of Louisville [Note: both numeral 0s in the userid)
H.E. Nuttall, Jr. (NUTTALL at UNMB), University of New Mexico
Peter R. Rony (RONY at VTVM1), Virginia Tech
Norman Rawson (RAWSON at MILVM1), IBM
Michael Cutlip (CHEGADM at UCONNVM), University of Connecticut
Heinz Preisig (HPREISIG at TAMKBS), Texas A&M
Jim Petersen (SCEF0003 at WSUVM1), Washington State University
J.P. O'Connell (CYKJYCS at NERVM), University of Florida
Richard LaRoche (LAROCHE at UIUCVMD), University of Illinois
Jim Hale (HALE at CLEMSON), University of Clemson
Professor Bryan (BRYAN at FREMP11), Ecole des Mines Paris, France
Cameron Crowe (CROWE at MCMASTER), McMaster University, Canada
Ram Lavie (CERRLRL at TECHNION), Technion, Israel
Avi Nir (CERRANAN at TECHNION), Technion, Israel
William Resnick (CERZRZR at TECHNION), Technion, Israel
Peter Cummings (PTC at VIRGINIA; CSNET userid), University of Virginia

Contact persons:

Carl P. Jefferson, University of Nevada-Reno
Kent S. Knaebel, Ohio State University
Ralph E. White, Texas A&M University
Bradley R. Holt, University of Washington
Ulrich Suter, MIT

CONFESSIONS OF AN ELECTRONIC MAIL USER

I have a BITNET userid (Rony at VTVM1) and have no difficulty answering BITNET messages sent to me by colleagues. Unfortunately, I have not used our IBM CMS operating system for years and am having trouble finding time to wade through the rather terse operating system and BITNET user manuals, experiment with the commands, and learn how to originate messages directly from stored files. Like many of my CACHE and CAST colleagues, the press of other commitments has interfered with my good intentions to become proficient with electronic mail, in this case, BITNET.

ELECTRONIC MAIL IN THE CLASSROOM: A TEACHING TOOL FOR THE FUTURE

Electronic mail systems can be used for a variety of non-traditional tasks by EDUNET members and suppliers. If your institution has electronic mail facilities, the following article describes three applications. If your school does not have an electronic mail system, EDUNET membership enables you to explore the potential benefits and to experiment with several systems. (See box for mail systems available through EDUNET.)

by Allison Chisolm
EDUNET Intern

With expanded use of electronic mail, instructors have begun to use these systems as tools for innovative teaching. Rutgers University, Case Western Reserve University, and Yale University have each utilized institutional electronic mail systems in innovative classroom experiments.

Rutgers University

In the fall of 1980, Lawrence A. Welsch, while a full-time technical staff member at Bell Labs, taught a software engineering course at Rutgers. To use his time more effectively, he employed the school's 24-hour electronic mail system resident on a DEC-20 as the course's primary mode of communication outside the three class hours per week.

Welsch instructed students to access an electronic bulletin board at least once every 24 hours to check for assignments and class announcements. He also encouraged them to submit helpful suggestions or information. If a student missed class, the bulletin board provided a permanent record of assignments, lecture topics, and outside reading.

Summarizing his experience in an article in Communications of the ACM, Welsch concluded that the quality of student/teacher interaction was greatly enhanced by the use of electronic mail. Students could ask questions outside class and receive almost immediate feedback. After assignment files were submitted, Welsch could insert comments electronically in the text before returning it. Copies of assignments applicable to the work of another project could be transmitted quickly and easily to each student involved.

Grading also became a more interactive process as electronic mail reduced the time lag between submission and return of homework. Because both student and professor could respond immediately, an assignment's value could be realized with the work still fresh in the student's mind.

Student fear that reliance on an electronic system would widen the communications gap between student and teacher proved unfounded. From a student poll made at the end of the semester, Welsch concluded that the enthusiasm for electronic mail was "somewhat overwhelming." Fifteen out of 22 respondents stated emphatically that "electronic mail should be considered a teaching tool regardless of subject matter." Once everyone gained a basic familiarity with the mail system (Welsch sent and received more than 1680 messages over the course of the semester), it proved an excellent way to learn from others. Overall, students considered electronic mail use a positive influence upon the course.

Case Western Reserve University

Paperless Homework, a research project at Case Western Reserve, has been in testing stage this year, with full implementation planned for September. Using 48 DEC 350 microcomputers, students in the Case Institute of Technology begin homework on floppy disks used as scratch pads, then turn work in to the electronic mailbox on their professor's resident disk. The professors then read their "mail," grade assignments, and return them with comments.

To avoid a last minute crunch for terminals before deadlines, the micros are part of a laboratory run like a chemistry lab session. Students are scheduled for three-hour periods on the terminal and may sign up for additional time 24 hours in advance. Onsite printing is available via one dot-matrix printer for every four micros. In September, high quality final copies can be made on a laser printer off a VAX 11/730 connected to the micros via an Ethernet local area network.

Yale University

In the fall of 1982, Yale formalized a course communication system similar to Welsch's at Rutgers, which also included shared disk space for common storage. Professors may access three designated disks on the IBM 4341 to store instructional files and programs as well as records of assignments and homework files. Used in conjunction with the electronic mail system, a Class disk, an Instructor disk, and an Electronic Homework facility are tailored to the needs of each class and act as a repository for class news, student questions, and submitted work. While primarily used in the hard sciences, instructional disks are currently incorporated in approximately 100 classes spanning all departments and disciplines.

Class disk usage extends the instructor's ability to communicate by providing additional class notes and storing the course statement of purpose. Accessible to registered students only, the disks act as a form of reserve reading. The Instructor disk, used jointly with the Electronic Homework facility, holds material exclusively for the professor's perusal.

Yale professor of anthropology Timothy Weiskel sees computers providing a useful teaching environment with the mail system as a supplementary tool, not a substitute for classroom teaching. He sees one advantage of the Class disk as the user's ability to automatically invoke menus for several kinds of assignments. Student preference and the amount of time spent on various programs can be evaluated for future course improvements.

Yale's Computer Center invites faculty to meet early each semester to learn about the computerized services as well as to assess future needs for computing in the classroom.

If your institution is interested in experimenting with local or national electronic mail, contact EDUNET at 609 734-1878; via MAILNET or BITNET: DAMORE @ EDUCOM.

Reprinted from EDUNET News, Fall 1984, pp. 3 & 4.

Computer-based Electronic Mail and Conferencing Systems at EDUNET Supplier Institutions*

Carnegie-Mellon University	*MS*, a standard mail system that can be tailored to suit individual needs; runs on a DEC-10 mainframe under the TOPS-20 operating system
University of Chicago	*MM (Mail Manager)*, a standard mail system running on a DEC-10 mainframe under the TOPS-20 operating system
	COM, a sophisticated mail and conferencing system running on a DEC-10 mainframe under the TOPS-20 operating system
City University of New York	*Yale Execs*, a set of interrelated exec files, under IBM's VM/CMS operating system, that provide mail functions and an interface to BITNET, an international network
University of Colorado	*VAXMAIL*, the standard DEC mail system on a VAX minicomputer under the VMS operating system
	MATRIX, a relatively new, sophisticated, menu-driven mail and conferencing system running on a VAX minicomputer under the VMS operating system
Cornell University	*Cornell Mail*, a Cornell-developed mail system on an IBM 3081 mainframe under the CMS operating system
Dartmouth College	*DCTS Mail*, (Dartmouth College Time Sharing), Dartmouth's own mail system on a Honeywell mainframe running the DTSS operating system
University of Delaware	*MSG*, a flexible mail system, oriented to memo-style communications; runs on a Burroughs with the MCP operating system
	RDMAIL, a standard electronic mail system on a DEC-10 mainframe under the TOPS-10 operating system
MIT	*Multics Mail*, a standard mail system, developed specifically for Multics, running on a Honeywell mainframe
MERIT: University of Michigan & Wayne State University	*CONFER*, a conferencing and messaging system designed for group decision making, discussions on a common topic, and personal communications; runs on a Amdahl under the MTS (Michigan Terminal System) operating system
NJ Institute of Technology	*EIES* (Electronic Information Exchange System), a powerful, sophisticated mail and conferencing system running on a Perkin-Elmer minicomputer
University of Southern California	*Hermes*, a sophisticated mail system that has many advanced features and can be customized for individual tastes and needs; runs on a DEC-20 under TOPS-20
Stanford University	*CONTACT/EMS*, a standard memo-type messaging system that interfaces to the powerful WYLBUR text editor and to the data base management facilities of SPIRES; also includes MAILNET and BITNET network interfaces; runs under WYLBUR on an IBM 3081 mainframe
University of Stockholm Computing Centre-QZ	*COM*, the powerful, and sophisticated mail and conferencing system on DEC-10s; portable version, PortaCOM, runs on various hardware/software systems
University of Wisconsin-Madison	*MACC Mail*, Wisconsin's own standard electronic mail system on a Sperry 1100 running the EXEC operating system
Yale University	*Yale Execs*, a set of interrelated exec files under IBM's VM/CMS providing mail functions and an interface to the BITNET network
GTE Telenet	*Telemail*, a electronic mail service for private messaging offering many advanced features, including bulletin boards, auto-delivery, and local account administration

*not an exhaustive list.

A TRANSPORT & THERMODYNAMIC PROPERTIES PACKAGE FOR PERSONAL COMPUTERS -- TTPGL

Hardware: IBM PC/XT/AT (or compatibles), TRS 80

Programming Language: FORTRAN IV

Operating System: PC-DOS 2.10 or higher
CP/M 2.24 or higher

Memory: 256K or 64K

Input Data Format: Interactive, Free Format

Documentation:

1. Shyu, A.K., M.S. Thesis, Fall 1984, Lamar University, Beaumont, Texas

2. Shyu, A.K., and D.H. Chen, "A Transport and Thermodynamic Properties Package for Personal Computers," paper 65, the 189th American Chemical Society National Meeting, April 28-May 3, 1985, Miami Beach, Florida (I&EC Division).

Description:

The transport and thermodynamic properties package TTPGL is applicable to both mixtures and pure components. New techniques developed in recent years such as the method of Teja and Rice for the prediction of thermal conductivity of liquid mixtures were built into the package. The user can estimate diffusivity, thermal conductivity, viscosity, density, heat capacity, enthalpy, and surface tension over a wide range of temperatures and pressures. The Peng-Robinson equation of state is used to estimate the phase equilibria and thermodynamic departure functions for mixtures. If some physical constants (used as inputs) are not available, the group-contribution subroutines are invoked. The package is interactive and suitable for personal computer-based engineering/instruction.

Cost: $200.00 (Executable Module + Documentation)

Notes: The program now distributed is the updated version, capable of handling 15 components and estimating polar liquid systems by mixing rules. Improvements currently under way are the usage of activity coefficient approach, addition of entropy estimation, and input of data from data files.

Contact: Dr. Daniel H. Chen
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Beaumont, TX 77710 Tel. (409) 880-8786

MATRIX -- MULTI PURPOSE PROBLEM SOLVER FOR IBM PC

Sung Kuk Soh
University of Detroit

MATRIX is a stand alone interactive program to manipulate matrices and systems of linear and nonlinear equations. Expressions can be programed similar to what one would write on paper. It has 63 built-in functions including trigonometric, exponential, statistical, gamma and error functions, Jacobian and Hessian. One can add user-defined functions so that it can be used as a programmable calculator whose entries may be matrices as well as real numbers. In the area of numerical integration, Romberg, Trapezoidal, Simpson, Gaussian quadrature and fourth order Runge-Kutta integration are supplied. Systems of linear and nonlinear matrix equations are solved by pivoted Gauss-Jordan elimination, Crout elimination, Newton-Raphson method, and Runge-Kutta integration. Iterative methods can be programed and one-dimensional optimization is built-in.

Hardware: IBM PC or MS-DOS computer with a disk drive and 128 K or more RAM.

The MATRIX program can be ordered for $50 from Soft-Tech Inc., 14640 LaBelle, Oak Park, MI 48237.

CACHE: A PROGRAM FOR INTERACTIVE CONTROL SYSTEM ANALYSIS AND DESIGN WITH A PERSONAL TECHNICAL WORKSTATION

Bruce H. Krogh* and Charles P. Neuman**

Department of Electrical and Computer Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
*** (412) 578-2472**
**** (412) 578-2460**

SUMMARY

CACHE has been designed, implemented and applied as an interactive *educational* software package for control system analysis and design. CACHE is a PASCAL program presently operating in a networked UNIX environment on 15 Hewlett-Packard HP9836 personal technical workstations in the Department of Electrical and Computer Engineering at Carnegie-Mellon University (CMU). Each workstation includes a 32-bit computer with 2 megabytes of memory, two 15 megabyte Winchester disc drives, two floppy disc drives, a locator pen and tablet, a hard copy thermal printer, and network connections to a plotter and a VAX 11/780 computer. CACHE's binary code currently requires 368 kilobytes of memory. Additional memory is allocated dynamically for data structures created during a user session.

Since computer-aided analysis and design have become essential ingredients of control engineering, it is imperative to provide control engineering students with accessible and modern computer resources. Many available commercial packages for control system analysis and design have been created for mainframe computers and large-scale production runs. Software for personal technical workstations is ideally suited for a modern educational environment because speed-of-response overrides the need for the student to perform large-scale computations. Our HP9836 personal technical workstations meet the needs of engineering students for rapid, interactive feedback in problem-solving and design sessions, without sacrificing computational power and graphics capabilities. In the Department of Electrical and Computer Engineering at CMU, moreover, these personal technical workstations are being used throughout the undergraduate and graduate curriculum. Familiarity with the computing environment is reinforced throughout our educational program and the *learning curve* for applying CACHE is thereby minimized.

CACHE was conceived in 1983 to provide undergraduate and graduate engineering students with comprehensive computational and graphics tools incorporating both classical and modern control engineering methodologies. Developed in a sequence of two senior honor's projects for course work, coherence and consistency of the user-interface and data structures were primary considerations. The *menu-driven* hierarchical command structure of CACHE aides the student in proceeding systematically through the steps of data and feedback control system analysis, design, and evaluation. The functions of the program are decomposed into four subsystems: *editor, filer, calculator* and *plotter.* Database management and file handling are accomplished in the editor and filer subsystems. The user can enter models of multi-input, multi-output systems by defining state-space or transfer function matrices, and construct feedback systems with the block diagram editor function. The calculator provides a vast library of computational routines for operations on polynomials, matrices and systems, including: PID controller design, computation of resolvant and state transition matrices, tests for modal controllability and observability, linear state-variable feedback controller design, and solution of algebraic Riccati equations for optimal LQR design. Since engineering students are the target users of CACHE, standard algorithms have been implemented to provide computationally efficient solutions to design problems involving low-order systems. The plotter creates and displays time and frequency responses, pole-zero and root-locus plots, and Nichol's phase-magnitude charts. The locator pen can be used to obtain the loop gain corresponding to any point on the root-locus plot.

The structure of the hierarchical database defines linear, time-invariant, dynamic physical systems by two primative data structures: matrices for state-space models and polynomials for transfer function models. Dual representations of all systems are maintained in both the time and frequency domains to reinforce understanding of the relationships between classical and modern control methodologies. Polynomials are stored by both roots and coefficients, regardless of the initial entry mode. Continuous-time and discrete-time systems are supported, including the step-invariant transformation of analog models into digital models. Linked-lists are used throughout the database to circumvent fixed dimensionality constraints.

CACHE has become a viable tool for the students in our undergraduate and graduate control engineering courses at CMU. CACHE has eliminated the tedium of routine algebraic and numerical calculations in traditional control engineering problem-solving and design. The availability of our truly interactive control system analysis and design software on a dedicated personal workstation is exciting the interest of our engineering students, and enhancing their learning experiences.

The complete paper appears in:

J.M. Mason, C.P. Neuman, and B.H. Krogh,
"CACHE: An Interactive Control System Analysis and Design Package,"
IEEE Transactions on Education,
Vol. E-28, No. 3, pp. 143-149, August 1985.

LIST OF CHEMICAL ENGINEERING DEPARTMENTS SUPPORTING CACHE

Last fall, CACHE solicited universities for funds to carry out on-going CACHE activities and to provide seed money for new projects. Departments providing support for the 1985-87 period, as well as for the 1984-86 period, are as follows:

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

Preliminary Design and Economic Analysis

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

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

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

CACHE PROCESS DESIGN CASE STUDY VOLUME 2

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

Preliminary Design and Economic Analysis

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

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

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

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

CACHE PROCESS DESIGN CASE STUDY VOLUME 3

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Documentation:

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2. *User's Manual*
3. *Instructor's Manual*
4. *Module Writer's Manual*
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Videotapes (VHS Format):

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<u>Modules</u>

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CAST/CACHE

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Editors: **Arthur Westerberg**, Carnegie-Mellon Univ. **Henry H. Chien**, Monsanto Company

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