CACHE NEWS

News About Computers In Chemical Engineering Education

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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 projects 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 the CACHE Newsletters. Individual inquiries should be addressed to

CACHE Corporation, Room 66-309
77 Massachusetts Avenue
Cambridge, Massachusetts 02139

CACHE TRUSTEES AND MEMBERS

CACHE NEWS

The CACHE News is published one or 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 address listed above.

CHEMI (CHEMICAL ENGINEERING MODULAR INSTRUCTION) PROJECT

The first phase of the CHEMI Project was successfully completed with the transmission of approximately 230 modules to the AIChE's Division of Continuing Education. Each module, which is 15-40 pages in length, and treats a single topic which would be the subject of a 1-3 hour lecture, contains in addition to the subject content an instructor's guide, and solved homework and study questions. The modules can be used for self-study, remediation, and as lecture and textbook supplement. The modules are grouped into six subject areas under the editorships of:

Ron Gordon	-	Transport
D. Himmelblau	-	Mass and Energy Balances
S. Fogler & Billy Crynes	-	Kinetics
J. Calo & E. Henley	-	Stagewise and Mass Transfer Operations
B. Goodwin	-	Thermodynamics
T. Edgar	-	Control

The modules will be "clustered" into groups of 5-8 when published by the AIChE in a symposium-volume format. Single-module sales are also envisioned.

The project has recently received additional funds from NSF to produce a set of modules for design topics, and to complete, evaluate and update existing materials. Electronic dissemination via micro-computer disks is envisioned. The continuation of the CHEMI Project will be under the direction of David Himmelblau.

NEW COMPUTER PROGRAMS TO BE MADE AVAILABLE

Professors Seider and Westerberg announced at the CACHE Representatives' dinner in San Francisco that a number of new computer programs will be made available for use in 1980. The programs are:

(1) RADFRAC - a very powerful and versatile column program by Joe Boston (ASPEN Project, MIT). It can simulate and optimize the performance of a distillation or absorption column. It is very fast and very reliable.

(2) A suite of five reactor programs by Bruce Finlayson (University of Washington) and Arvind Varma (Notre Dame). These include:
- REACOLL and REACFD, which solve the radial dispersion pseudo-homogeneous model for the fixed-bed reactor,
- ETAPHI and CATEFF, to compute catalyst effectiveness factor versus Thiele modulus curves, and
- SSTR, which computes concentration and temperature profiles in an axial dispersion model non-adiabatic tubular reactor.

Professor Finlayson's programs (REACOLL, REACFD, and ETAPHI) have been tested in actual classroom use for over five years, while Professor Varma's programs have been used largely in research.

(3) ASCEND and EROS - two programs by Arthur Westerberg (Carnegie-Mellon University). ASCEND is a suite of interactive design programs, useful in teaching the senior design class. ASCEND includes six variations of the flash unit, a shortcut distillation column and a shortcut absorber. VLE and enthalpy data can be estimated using the Wilson equation, Praunitz-Chueh or ideal. ASCEND also has a fitting routine to fit binary Wilson parameters to actual data. EROS is a program to analyze and optimize a network composed of simple heat exchangers, stream splitters and mixers. It is useful for teaching students the user convenience possible in flowsheeting systems. Both programs are documented with an extensive online "HELP" system and are designed to require a minimum of classroom instruction to use. Both are also supported by a file handling/data retrieval system so runs may be interrupted, edited, and continued the next day.

One of the possible mechanisms whereby faculty members can check the programs out at little cost may be via EDUNET. EDUNET is a network of university computers accessible remotely over the TELENET communications network. What this means for you is that you can usually access the university computer on which the program resides using a local phone call, not unlike you currently can access FLOWTRAN over the United Computer Systems network. Costs should be much less over EDUNET, particularly for access using a slower (300 band) terminal. Another possibility is for user to directly obtain an account with the home computer center for the program. More information as to access will be available later.

PPDS JOINS CACHE NETWORK SERVICES

At its meeting in St. Louis in May, 1979 the CACHE Board of Trustees approved the Task Force plan to lease the PPDS physical property retrieval and estimation program from the British Institution of Chemical Engineers. Contractual details are being ironed out with I. Chem. E. - PPDS for a two-year lease to begin in late 1979. The program is distributed in source code and installation is expected to take less than a day.

Yet to be identified is the computer on which the program will be installed. There are at least two possibilities: (1) the UCS network coresident with FLOWTRAN or, (2) on an appropriate EDUNET supplier university computing center over the TELENET network. Resolution of this matter in consultation with the Program Distribution Task Force is anticipated in the near future. Comments from reader would be appreciated. Write Rudy Motard.

The PPDS system provides 18 physical constants and 15 variable properties for each species stored in the data bank. The variable properties are temperature- and pressure-dependent. Properties of mixtures are also generated for the variable properties. The CACHE version will provide a 50-compound subset of the PPDS commercial data bank. Properties may be tabulated at a computer terminal or may be called from a design program through a FORTRAN callable interface.

Financial support for the project has been generously provided by duPont and Simulation Sciences, Inc. In the meantime several additional companies in the U.S. who are commercial users of the system have been approached for additional support, either to extend the two-year lease period, or, to allow CACHE to purchase its version outright.

MICROCOMPUTERS AND PROGRAMMABLE CALCULATORS TASK FORCE

During the past year, the main effort of the Task Force has been to obtain federal funding. The basic thrust of the proposal is to develop a supervisory system and a number of interactive programs for use on microcomputers such as the PET and APPLE. This proposal is still pending. A few trial program modules in chemical reaction engineering were developed by students at the University of Michigan, and these programs are stored on cassettes for use on the Commodore PET 2001. During the coming year it is hoped that more faculty will be involved in developing and exchanging the prototype programs. Anyone interested in joining this Task Force or in exchanging or borrowing a sample program cassette should write to Prof. H. S. Fogler at the University of Michigan.

In the area of hand held programmable calculators, Professor William Kroesser has accepted the sub-chairmanship of the Task Force. He will be preparing a list and short abstract of available calculator programs in chemical engineering. He will also investigate preparation of a book containing calculator program listings, descriptions, and limitations of the programs and equations in chemical engineering similar to the series currently appearing in Chemical Engineering Magazine (e.g. Chem. Engrg. July 30, 1979, p. 79).

PROGRAM AT THE ASEE ANNUAL MEETING, 1979

A progress report on the activities of CACHE was presented. The specific activities included the CHEMI teaching modules project, program library on a computer network, and real time computing by the following speakers, respectively:

Ernest J. Henley, University of Houston
Arthur W. Westerberg, Carnegie-Mellon University
Duncan A. Mellichamp, University of California-Santa Barbara

GRAPHICS SURVEY

There is presently quite a bit of interest in computer graphics so the CACHE Computer Graphics Task Force recently completed a survey on computer facilities and usage in chemical engineering departments. Some of the pertinent results of the survey are as follows:

1. Of the 154 departments of ChE, 87 responded to the survey (survey mailed mid-March and returned by May 1 with followup mailing by July 1).
2. Of the 87 departments, 67 indicated availability and/or usage of graphics devices. Slightly over half of these departments own the equipment, the remainder being operated by computation centers or a college of engineering. 58/67 departments had access to interactive terminals, mainly Tektronix. This is to be compared with 14 departments responding positively to a survey in 1976.
3. In teaching, there are interactive applications reported in dynamics and control simulation, design, kinetics, heat transfer, thermodynamics, distillation and stoichiometry, as well as simple plotting. In research, much of the usage is in XY plotting and preparation of figures for manuscripts; otherwise, the same areas as noted above have graphics applications.
4. Three of the four proposed Task Force activities were well-received (inventory of software, workshops/technical sessions, and applications notes); the network idea was not affirmed.
   Other ideas advanced included micro-minicomputer applications of graphics, developing specific software, the transferability issue, formation of a Plato users group, equipment surveys, and use of graphics classrooms. One respondent suggested that documented use of graphics in industry would assist his department in acquiring facilities.
5. Several new members of the graphics Task Force have been identified through the survey. If you are interested in participating in the Graphics Task Force activities, write to Thomas F. Edgar, the Department of Chemical Engineering, The University of Texas at Austin.

The survey results are presented below.

CACHE Computer Graphics Survey 8/1/79

UNIVERSITY	TERMINALS, OTHER SUPPORTS	RESEARCH	TEACHING	DESIRED APPLICATIONS, SOFTWARE
Akron	T			
Alabama	CALCOMP			
Alberta	T4013* HP2648*	Data Display, controller design	Control	Control systems displays, transferable graphics programs for minis
Arizona	T4010	No	No	
Arizona State	T4010*	No	No	

UNIVERSITY	TERMINALS, OTHER SUPPORTS	RESEARCH	TEACHING	DESIRED APPLICATIONS, SOFTWARE
Bucknell	T, APL	XY Plotting		Interactive control program
Calgary	CALCOMP*, T4010, 4013, 4014, considering DISSPLA	Figure preparation	XY Plotting	Honeywell Multics Graphics
UC-Berkeley	CALCOMP	XY Plotting	No	
UC-Davis	T4012*	Passive Graphics	No	What software is available? Uses in control, design and kinetics. They have a graphics classroom but no software.
Cal. Tech	PDP8, 11-VT55* HD*, T	Data Display	Process control Data analysis	3D graphics
Carnegie-Mellon	HP2648*, many others	CAD	No	
Case W.R.U.	T4015*	APL graphics	APL graphics	
Clarkson	CALCOMP, CRT	No	No	
Clemson	T4070*	Computer Movies CALCOMP preview		
Colorado	T4013*, 4652* IMLAC, PDP-11 DIGRAPH (CDC)	General plotting, Control research	XY Plotting, Control system design	Mini-micrographics, interacting programs for simulation and control
Connecticut	T4014*, Plato	Flowsheeting, real-time data acquisition	Plato (reaction engineering)	simulation programs in BASIC
Cornell	Plato acquire*			
CUNY	CALCOMP, APL T4013, 4631	Interactive Use		
Delaware	T*/T, HP, Plato (Many)	Yes	Plato, Use with class monitors	
Florida	PDP11*, G, T4013	Data display, phase diagrams	No	Flowsheet plotting, micro interfaces
Georgia Tech.	CALCOMP	XY Plotting	No	
Idaho	PDP-11 plotter			graphics capabilities
Iowa	Versatek, T, HP			
Kansas State	VT-55			3-D phase diagrams, McCabe Thiele
Kentucky	T4051*, T4631*, Lear-slegler	Yes	Yes	chemical engineering software
Lehigh	None			
La. Tech.	T4006*, T4051, T4081	No	Process Control	Kinetics, unit operations design programs
McMaster	Versatec (not interactive)	No	XY Plotting	Limited by Univ. computer
Michigan	DEC339, T4010, 4012, (IG Software)	flow sheeting development	Games, simulation in kinetics	Inventory of available equipment?
Minnesota	T*	process control and design	controller design	
Mississippi State	G4800	Yes	Yes	

UNIVERSITY	TERMINALS, OTHER SUPPORTS	RESEARCH	TEACHING	DESIRED APPLICATIONS, SOFTWARE
Missouri (Rolla)	CALCOMP, CRT'S	Yes	No	
MIT	T*, CALCOMP*	Yes	No	Contour pkg., hidden line-3 dimensions
Nebraska (Eng. Mech.)	G, CALCOMP 15 CRT'S COMPLOT	Design		Tridem
New Brunswick	MINC-11*, G	data plotting		
New Mexico	HP*, T* (to be acquired)	XY Plotting	Simulation, Dynamics	
N. C. State	ICS 8001 (color)*, Decwriter*	pilot plant data analysis, display		Plato users group report quality graphics
Northwestern	T4010*, IMLAC	process synthesis	CAD	process control software
Notre Dame	T* (acquiring one)			Differential
Nova Scotia	T4051*, 4662*			
Ohio State	DEC VT-15* CALCOMP, HP*	CAD	Use in teaching larger classes?	Interact with ACM mini-computer applications program.
Oregon State	T4014*, 4662* T4010*, Gerber 1022	2, 3 dim. plotting	Computer aided flow sheeting, material energy balance	
Pennsylvania	VT-11, CALCOMP, PDP 11/34*, RAM TEK, Vector General	Analysis of fermentation kinetics	Fermentation kinetics Demon.	Curve fitting data display
Pittsburgh	T4010, C400			
Princeton	T4013* (2)	Control	Yes	
Purdue	T4006*, CALCOMP	Process Design	No	
Queens	plan to acquire			
Rhode Island	plotter	Figure preparation		
Rochester	T* (on order) Pet*	Dynamics	Soph. Lab. Dynamics & Con.	
RPI	IMLAC, T4014 IBM 3277A	Yes	Heat Transfer Process Control	Multivariable control software
Saskatchewan	HP* (2)	Plot Streamlines Isovels	XY plotting	
S. Carolina	DEC*, MINC (on order)	Real time data collection and display		Flexible plotting programs
S. Florida	T4001*	yes	yes	
SUNY (M.E. Dept.)	T4010*, T4006*	Design	Graduate course in CAD	3-D orthographics pkg.
Tennessee	T, CALCOMP	Simulation, data analysis		Software evaluation
Texas	T4014*, T4662* Vector General	Control, Simulation, CAD	Control, Simulation	Multivariable controller pkg.
Texas A&I	XY Plotters*	Yes	Yes	What software is available?

UNIVERSITY	TERMINALS, OTHER SUPPORTS	RESEARCH	TEACHING	DESIRED APPLICATIONS, SOFTWARE
Toledo	T4051, T4014 (not used by ChE)			
Toronto	Yes	limited	no	Plato users group
Tufts	C300*	Yes	Distillation	
Tulane	Plotter			
Tulsa	CALCOMP	XY Plotting	XY Plotting	
Washington (St. Louis)	T4010* (plan to obtain), DEC-10, IBM 360/370	process synthesis data analysis	CAD	PLATO, Fogler's reaction programs, Rosenbrock's control package
Washington (Seattle)	T* (to be acquired)		XY Plotting	
Waterloo	CRT*	XY Plotting	No	Graphics examples, list of available software
Wayne State	PDP-11, Evans-Sutherland	XY plotting	No	
Wisconsin	T4006*, Tr010*	CAD	CAD	process design software
Utah	T4013	No	No	Needs guidance in terminal purchase
Youngstown State	HP*			

Key:

* - Owned by Ch.E. Department
T - Tektronix
C - Computek
G - Gould
HP - Hewlett-Packard

CACHE PUBLICATIONS

CACHE Computer Graphics in Chemical Engineering Education, 66 pages (June 1978); Carnahan, Mah, Fogler.

CACHE Monograph Series in Real-Time Computing, D. Mellichamp, ed.; available from Brice Carnahan, University of Michigan, Ann Arbor, Michigan 48109.

I. An Introduction to Real-Time Computing (1977)
II. Processes, Measurements, and Signal Processing (1977)
III. Introduction to Digital Arithmetic and Hardware (1978)
IV. Real-Time Digital Systems Architecture (1978)
V. Real-Time Systems Software (1978)
VI. Real-Time Applications Software (1977)
VII. Management of Real-Time Computing Facilities (1979)
VIII. Process Analysis Data Acquisition, and Control Algorithms (1979)

Exercises in Process Simulation Using FLOWTRAN, 209 pages (1977); J. Peter Clark, ed.

Flowtran Simulation - An Introduction, 2nd ed., 1977; Seader, Seider and Pauls; available from Ulrich's Bookstore, 549 East University Avenue, Ann Arbor, Michigan 48104.

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CACHE Guidelines for Computer Networks, 25 pages (June 1974); Seider, Hughes, Mah, Phillips, Seader, Shannon, and Westerberg.

Real Time Task Force Report, 52 pages (October 1973); Elzy, Evans, Gallier, Mellichamp, Moore, Schmitz, Seborg, Smith, Weaver, Westerberg, Williams and Wright.

CACHE Guidelines for Large Scale Computer Programs, 16 pages (February 1973); Seader, Evans, Hughes, Seider, and Shannon.

Computer Programs for Chemical Engineering Education; available from the Sterling Swift Publishing Co., P.O. Box 188, Manchaca, Texas 78652.

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Stoichiometry	241 pages	Sept. 1972	E. J. Henley
Kinetics	388 pages	Sept. 1972	M. Reilly
Control	240 pages	Sept. 1972	A. Westerberg
Transport	418 pages	Sept. 1972	R. Gordon
Thermodynamics	400 pages	Sept. 1972	R. Jelinek
Design	400 pages	Sept. 1972	R. Jelinek
Stagewise Computations	500 pages	Sept. 1972	J. Christensen

CACHE Physical Properties Data Book, 35 pages (August 1972); Motard, Samuels, Hall, O'Connell, Seider, Wilson.

Real Time Digital Computer Systems in Undergraduate Education - St. Louis AIChE Meeting, CACHE Symposium, May 24, 1972, 24 pages (May 1972); Elzy, Evans, Weaver, Westerberg.

Standards for CACHE Fortran Computer Programs, 35 pages (May 1972); Shannon, Grens, Hughes, Klaus.

Computer-Aided Chemical Synthesis - A CACHE Sponsored Symposium, 6 pages (February 20-25, 1972); Seader, Elzy.