

CACHE NEWS

**News About Computers
In Chemical Engineering
Education**

No. 9

October, 1978



PURPOSE OF 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.

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COMMUNICATION WITH CACHE

CACHE actively solicits the participation by interested individuals in the work of on-going projects. Anyone who wishes to learn more about current CACHE activities may contact any member or write to CACHE, Room 66-405, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139.

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.

CACHE PUBLICATIONS

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

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

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

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

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

CACHE Use of Flowtran on UCS, Richard R. Hughes.

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

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

Flowtran Simulation—An Introduction. 2nd ed., 1977; Seader, Seider, and Pauls; available from Ulrich's Bookstore, Ann Arbor, Michigan.

CACHE Monograph Series in Real-Time Computing. D. Mellichamp, ed.

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

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

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

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

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

CACHE ELECTS NEW OFFICERS

At the CACHE Semiannual Meeting held outside Philadelphia in June, Prof. David Himmelblau (University of Texas) was elected CACHE's new President. CACHE's new Vice-President is Prof. R. R. Hughes of the University of Wisconsin; and Prof. Richard Mah of Northwestern University has been elected incoming Secretary. CACHE's headquarters in Cambridge will continue to be directed by our Executive Officer, Prof. L. B. Evans of MIT. The officers welcome contacts from CACHE departmental representatives, from Department Chairmen, and from industrial associates for information and for comment on current and potential CACHE initiatives.

ELECTION OF CACHE TRUSTEES

The election of new Trustees to the CACHE Corporation will be held at the Corporation's annual meeting in November. The nominating letter should be accompanied by four copies of a 2-3 page summary of biographical information concerning each individual in the following format (for uniformity):

- (1) Name
- (2) Rank
- (3) Department, School, Address
- (4) Education and degrees
- (5) Teaching experience
- (6) Industrial experience
- (7) Consulting experience
- (8) Research and professional interests
- (9) Previous CACHE or CACHE related activities
- (10) Professional society activities

(11) Principal publications in last 5 years

Nominations should be addressed to:

Professor Richard R. Hughes
Engineering Experiment Station
University of Wisconsin
1500 Johnson Drive
Madison, WI 53706
(608) 263-1602

Deadline for receipt of nominations is November 7, 1978.

DINNER MEETING FOR CACHE REPRESENTATIVES

Arrangements have been made for CACHE to host a dinner meeting for CACHE representatives at the Americana Hotel in Miami on Tuesday, November 14, 1978. The discussion of future directions for CACHE at the last CACHE representatives' meeting in Philadelphia was very stimulating, and the next meeting should prove equally rewarding.

NEW TASK FORCE ON PERSONAL COMPUTERS

A new task force is being developed on the use of personal computers (e.g. TI-59, PET) in Chemical Engineering Education. The initial thrust of this project shall focus on the development of modules in Chemical Engineering design. In particular, we should be looking at the sizing of reactors, distillation columns, gas absorbers, filters, and other equipment one would find in the preliminary design of a chemical plant. The programs should be written so that one can rapidly size a distillation column with the sophistication that is somewhere between hand calculations and the full scale simulation of a distillation column using the IBM 360 computer. Once the various operations are sized, it is anticipated that the student could substitute in the appropriate data relevant to his process and design a complete plant within a matter of a couple of hours.

With the programmable calculators (computers) being utilized to eliminate the majority of time spent on hand calculations, the student using these modules will then be able to focus on the "synthesis" aspects of his process and perhaps allow him to be more creative in his solution. Anyone interested please contact Scott Fogler, Dept. of Chemical Engineering, The University of Michigan, Ann Arbor, MI 48104.

CHEMI PROJECT NEARS COMPLETION

The CHEMI Project, supported by the National Science Foundation and the CACHE Corporation, is producing over 250 single-topic, stand-alone modules spanning the entire undergraduate Chemical Engineering Curriculum. The project is about three years old and is nearing completion.

Both the AIChE and NSF are working on an agreement that the AIChE publish the modules and make them available. Expected first publication is February 1, 1979. Details on purchasing the modules, will be made available through the normal AIChE publications.

COMPUTER GRAPHICS/MICROPROCESSOR DEMONSTRATION

At the AIChE Annual Meeting, Miami, Florida (Nov. 13-16, 1978), the Computer Graphics and Real-Time Task Forces of the CACHE Corporation are sponsoring informal demonstration sessions on the use of microprocessors and computer graphics in chemical engineering.

The demonstrations are being coordinated with regular sessions sponsored by the new Division of Computing and Systems Technology, namely

Impact of New Development in Computer Hardware
Education in Process Control
Computers in Process Design and Control
Recent Developments in Control and Estimation

Participants who will be at the demo session in Miami include

1. Dr. Peter Rony (VPI) and Dr. Bob Furgason (Idaho)—demonstration of microprocessors
2. Tektronix—storage tube and raster color graphics terminals
3. Compeda—pipework design management system
4. Dr. Stan Sandler (Delaware) and Dr. Ron Andres (Princeton)—interactive graphics in ChE curriculum
5. Integrated Software Science Corp.—DISSPLA graphics output software
6. Foxboro—computer graphics in process control

There will also be a resource booth at the demo session with educational material on microprocessors and computer graphics.

Graphics equipment, microprocessors, and demonstration software provided by vendors and users will be made available to registrants at the Annual Meeting. The facilities will be open on Tuesday and Wednesday afternoons (2:00-5:30pm) and Wednesday and Thursday mornings (9 am - 12 noon).

CACHE SOLICITATION OF UNIVERSITIES

CACHE initiated a solicitation of universities in the Spring of 1978. This is the second general solicitation that CACHE has made, and it has been quite successful. As of the first of September, 1978, fifty-seven United States and seven Canadian schools indicated that they would be willing to subscribe \$200 to help fund CACHE activities. This response has been most impressive, particularly in view of the late date of the solicitation relative to budgeting for 1978-79.

If your own department has not yet contributed to this drive, why not take a minute of your time and talk your departmental chairman into initiating the necessary paper work.

We received 75 responses from the 140 Departments of Chemical Engineering in the United States and four from abroad. Of the 79 departments responding, 73 encouraged CACHE to create a library and 67 indicated possible participation.

Three of the programs were of high interest; PPDS, BALTAZAR, and the program for analysis of separation towers. Five more were of significant interest and four were of low interest. Respondents estimated expenditures of approximately \$15-\$20 per student and about \$250-\$425 per course.

CACHE LIBRARY OF COMPUTER PROGRAMS FOR CHEMICAL ENGINEERING EDUCATION AND RESEARCH

In April, Professors Warren D. Seider and Arthur W. Westerberg prepared a Prospectus to explore the possibility of creating a library of computer programs for use in chemical engineering education and research. Copies were sent to CACHE representatives at 180 chemical engineering departments to determine the potential usefulness of twelve programs and to computer networks to explore the feasibility of creating such a library at reasonable cost.

The library would reside on a large-scale computer and be accessed through a low-cost communications network. It would contain large

programs and data bases that are cumbersome to transport and install on inhouse computers, maintained and updated by their authors. In some cases, programs would continue to be augmented and upgraded in the course of research work. These programs may not be well-suited for use by students in homework, but would provide a vehicle for researchers to communicate in the development of new methods; for example, in process synthesis.

The CACHE library would consist of FLOWTRAN and several other programs; the twelve candidates presented in the Prospectus are:

1. **EROS** (A. W. Westerberg and J. V. Shah)—A program for quick evaluation of alternate energy recovery systems.
2. **UMIST Computer—Aided Control System Design Suite** (N. Munro, B. J. Bowland, L. S. Brown)—A suite of programs that allow on-line analysis, design, and simulation of control systems.
3. **Multicomponent, Multistage Separation Tower Analysis Program** (J. F. Boston)—A program to stimulate separation systems using distillation, adsorption, reboiled adsorption, and extractive distillation.
4. **MULTI-BATCH** (D. W. T. Rippin, G. J. Forder, R. E. Sparrow)—A computer package for the design and rating of multi-product batch plants.
5. **BALTAZAR** (R. L. Motard, V. Mahalec)—A program for synthesis of flow sheets for continuous chemical processes.
6. **UNIFAC Computer Programs** (A. Fredenslund, J. Gmehling, P. Rasmussen)—Programs for computing vapor-liquid equilibria using the UNIFAC group contribution method and for simulation of distillation towers.
7. **PPDS** (Institution of Chemical Engineers, London, England)—A physical property data service.
8. **HARAD** (E. J. Henley)—Programs to analyze the safety, reliability, and availability of chemical processes.
9. **PDS** (J. Erbar)—A program to perform heat and material balance calculations for any process configuration.
10. **COAL2** (W. E. Schiesser)—Dartmouth National Energy Policy Model.
11. **TWOFAZFLOW** (F. R. Morris, T. W. F. Russell)—A program for calculation of two phase flow design parameters.

12. **DSS/2—Differential System Simulator** (W. E. Schiesser)—A program for integration of systems of ordinary and partial differential equations using the method of lines.

NETWORKING CONFERENCE

On September 28-29 we convened an NSF-sponsored conference to consider "How Can the Chemical Engineering Discipline Best Utilize Networks for the Sharing of Computer-Based Resources in Research and Teaching." The conference was organized by CACHE and EDUCOM, The Interuniversity Communications Council (P. O. Box 364, Princeton, New Jersey 08540). Professors Seider and Westerberg, Ronald Segal and Carolyn Landis of EDUCOM prepared the proposal and organized the agenda.

The conference was attended by 25 persons including professors of chemical engineering, industrial researchers, representatives of EDUCOM and EDUNET (uses the TELENET communications network to communicate with several university computers), United Computing Systems, and Control Data Corporation. The sessions were entitled:

1. State-of-the-Art of Computing in Chemical Engineering: Instruction and Research Applications
2. Summary of Needs: Based upon the response to the CACHE Prospectus
3. Computing Options Available to Chemical Engineers
4. Network Plans and How They Might Satisfy the Perceived Needs
5. Experiences in Facilitating Use of Programs and Textual Material for Teaching and Research at Remote Sites

The conferees worked to develop an Action Plan for creation of the CACHE Library, the initial stages of which are presently being implemented. The entire Action Plan is included as part of a Final Report describing the Conference, copies of which will be available from CACHE and EDUCOM by the new year. We will describe the Action Plan in detail in the next CACHE Newsletter.

COAL CONVERSION PROCESS SIMULATION PROJECTS AT PURDUE AND LEHIGH UNIVERSITIES

Two parallel research projects have been in progress at these universities under DOE contracts since the spring of 1976 and continuing through the third quarter of 1979. The dual goals of these projects are:

- i) to develop steady state (Purdue) and dynamic (Lehigh) simulation programs which would be suitable for coal conversion process modeling and which would have unrestricted distribution
- ii) to apply these programs to study one or more selected coal conversion processes in a programmatic fashion

To date significant progress has been made both in the development of the program systems themselves and in their applications to coal conversion processing.

The components of the steady state simulation/design system that have been designed, implemented, tested and largely documented, include a process equipment simulation and information processing system, flowsheet material and energy balance programs, a physical properties estimation package, an equipment costing data bank, and a flowsheet graphics program. During the past year the formulation and literature review were carried out for a conceptual flowsheet of a COED based process which incorporates most of the key processing steps to be implemented in the Illinois Coal Gasification Group Demonstration Plant. Work in progress at the present time and projected to be completed under the current contract includes further additions to the simulation system and continued process modeling and flowsheet simulation case studies. For further information contact: Prof. G. V. Reklaitis, School of Chemical Engineering, Purdue University, W. Lafayette, IN 47907.

The general approach adopted for the dynamic simulation of coal-conversion plants is two-fold:

- 1) The development of a general-purpose FORTRAN IV program for the solution of systems of initial-value ordinary and partial differential equations (ODE/PDEs)
- 2) The application of this code to the dynamic simulation of a high BTU coal gasification plant as a concrete example.

The general purpose Differential Systems Simulator (DSS/2) is completed and documented at the present time. The dynamic models of the process sections are being documented as separate DDS/2 applications studies.

Using DSS/2 several major sections of the modified COED process have been successfully simulated. These include the RMP bulk methanation section, the COED type multi-stage pyrolysis plant, as well as the COGAS gasification system. The most recent application, the dynamic model of the gasification section, includes a cyclonic combustor and a char lift tube. The model assumes quasi-steady state for cyclonic combustor, lift tube, and gasifier gas phase but considers the detailed dynamics of the gasifier solid phase. For further information contact: Professors W. E. Schiesser and Fred P. Stein, Department of Chemical Engineering, Lehigh University, Bethlehem, PA 18015.

COMING EVENTS

Miami AIChE Meeting, November 13-16, 1978
Computers in Design and Control, W. D. Seider and L. C. McCune

Impact of New Developments in Computer Hardware and Software, R. S. H. Mah and D. Prater

Free Forum on Computing Technology, I. Rinard and R. Stanfield

Productivity in Programming Projects, N. E. Rawson and M. L. McGuire

Mini- and Microcomputers in Control, January 8-9, 1979, Islandia Hyatt House, San Diego, California. Contact: The Secretary, Computers in Control Symposium, P. O. Box 2481, Anaheim, CA 92804. (714) 774-6144

Houston AIChE Meeting, April 2-5, 1979
Optimal Allocation in Energy Networks, R. W. Pike and F. Pitts
Simulation of Fossil Fuel Related Processes, L. B. Evans and L. Joseph
New Developments in Process Analyses, R. S. H. Mah and A. W. Westerberg
Application of Improved Control Methods to Batch Processing, David Fraade
Control Systems for Energy Management/ Energy Conservation, James W. Lane and Thomas Tsai
Computer Control: An Industrial Case History, Eli Nisenfeld
Process Control Techniques, Jay Bailey
Distillation Column Control Strategies, Thomas F. Edgar
Computers in the Plant, Donald Griffin

12th Symposium on Computer Applications in Chemical Engineering, Montreaux, Switzerland, April 8-11, 1979.

Joint Automatic Control Conference (JACC), Denver, Colorado, June 17-20, 1979. Program Chairman: T. F. Edgar, Department of Chemical Engineering, University of Texas, Austin, TX 78712.

Summer Computer Simulation Conference, Toronto, July 16-18, 1979. Program Chairman: Leon Levine, Computer Science Department, University of California, Los Angeles, CA 90024.

"Computer Applications to Chemical Engineering Process Design and Simulation," Sponsored by I&EC Division of ACS at 178th National ACS Meeting, Washington, D. C., Sept. 9-14, 1979.

Session I: State of the Art (Review Papers).
Chairman: Prof. Robert G. Squires, School of Chemical Engineering, Purdue University, W. Lafayette, IN 47907

Session II: Modelling and Simulation of Industrial Processes. Chairman: Dr. Gary E. Blau, Senior Research Specialist-Math Applications Group, 1707 Building, Dow Chemical USA, Midland, MI 48640

Session III: Computational Techniques in Design and Simulation. Chairman: Prof. G. V. Reklaitis, School of Chemical Engineering, Purdue University, W. Lafayette, IN 47904

Session IV: Optimization and Control of Chemical Processes. Co-Chairman: Prof. Duncan Mellichamp and Prof. Robert Rinker, Dept. of Chemical Engineering, University of California—Santa Barbara, Santa Barbara, CA 93106

5th IFAC Symposium on Identification and System Parameter Estimation, Darmstadt, Federal Republic of Germany, September 24-28, 1979.