

# **CACHE NEWS**

**News About Computers  
In Chemical Engineering  
Education**

**No. 6**

**May, 1977**



## PURPOSE OF CACHE

CACHE was established to accelerate and coordinate the introduction of digital computation in chemical engineering education.

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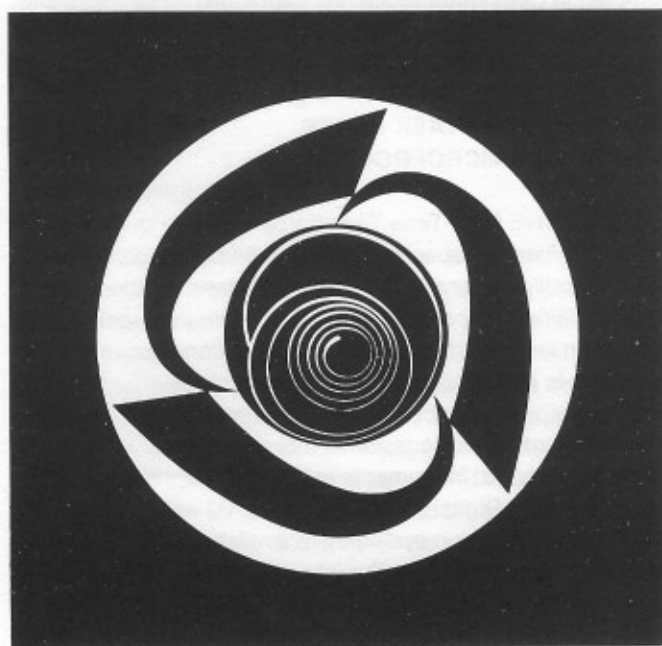
## COMMUNICATION WITH CACHE

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.

Material for publication in *CACHE News* is solicited from all sources. Submissions should be directed to CACHE at the above address or to the editor, Cecil L. Smith, Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803.

## CACHE NEWS



## CACHE RECEIVES INDUSTRIAL SUPPORT

CACHE has received three grants from industry during the past year: one each from Monsanto, Shell, and Exxon.

Monsanto provided \$8,200 for 1977 in continued support of the CACHE program to provide FLOWTRAN use by departments of chemical engineering at universities. This is the fourth year of support by Monsanto; previous awards have totaled \$29,000. In announcing the grant, Dr. James R. Fair, Director of Engineering Technology, expressed Monsanto's "best wishes to CACHE for another successful year in Chemical Engineering Education."

In January, Doris J. O'Connor, Senior Vice President of the Shell Companies Foundation, announced a grant of \$3,000 to the CACHE Corporation in support of its activities. This was the second award by Shell, with a previous grant of \$4,000 in 1975.

The Exxon Education Foundation has provided a grant of \$4,000 to be administered by M.I.T. for use in connection with the preparation of educational materials by CACHE. Paul V. Smith, Manager of Educational and Scientific Relations at Exxon Research and Engineering Company, commented that Exxon was "impressed with the potential of the educational program CACHE has under way."

The industrial support is particularly valuable at this time as the CACHE Corporation is trying to become established and self supporting. The Development Committee, headed by Professor David Himmelblau, plans to approach a number of other companies for support in the near future.

## DATA BASE MANAGEMENT/PHYSICAL PROPERTIES TASK FORCE

This task force has been in a monitoring mode for the past year, keeping tabs on a rapidly developing international scene on data management in engineering and physical property data base projects. We expect to propose the installation of at least one property data base system on the CACHE computer network for academic use in 1977.

On the national scene, through our interface with the Machine Computation Committee (MCC) of AIChE (soon to become the Computer Technology Division) we have been privy to the activities surrounding the "Bob Reid data base project." A data base of physical properties and estimation parameters for several hundred chemical species will appear in the third edition of Reid & Sherwood (and Prausnitz) forthcoming from McGraw-Hill. This event has spawned interest in a national data base project, initially proposing to generate a species-property matrix of validated constants for 1000 ubiquitous pure chemical compounds. National Bureau of Standards (Dr. Howard White) has expressed interest in managing the project, which has been given the tentative name of Project Evergreen. Negotiations are continuing for AIChE to become the umbrella organization for industrial financial solicitation. Evan Buck of Union Carbide is the industrial spokesman and R. L. Motard of the University of Houston is the MCC liaison.

On the international scene several property data base projects are gaining attention: PPDS (Britain), JUSE-AESOP and EROICA (Japan) and DECHEMA (West Germany). Most of



these are commercial ventures and would only be accessible to CACHE on a negotiated financial plan for strictly academic use.

The PPDS package of the British Institution of Chemical Engineers jointly with Imperial Chemical Industries is a combined retrieval and design property generation system. It contains physical constants and estimation parameters on 400 species. One can retrieve properties through an interactive terminal or interface design programs through a series of subroutine calls. Discussions have been held on CACHE participation.

The DECHEMA system is similar to PPDS and is based on a package developed by the Friedrich Uhde Company. It contains 350 species and a variety of estimation methods as does PPDS. A document retrieval system included in the package lists abstracts of pertinent literature references on data, properties and estimation procedures. This group has not been approached regarding CACHE involvement.

Finally, we have close liaison with the Japanese systems at the Japan Union of Scientists and Engineers (JUSE) and at the University of Tokyo (EROICA). The latter is especially interesting because it allows the retrieval of properties on 5000 pure chemical species. If the properties of specific compounds do not exist in the data base an estimation procedure based on chemical structure input is invoked.

## **CACHE REAL TIME TASK FORCE ACTIVITIES**

The CACHE Real Time Task Force has been re-assessing its role and structure since the chairmanship of the committee passed to Dr. J. D. Wright of McMaster University from Dr. D. A. Mellichamp of the University of California, Santa Barbara, last spring. At the present time the structure of the Task Force is being updated to appoint some new members and affiliate members in order to reflect the changes in technology and the interests of the various people involved. The objectives of the Task Force are being reformulated and directions for new activities are being defined. The Task Force intends to maintain a continued presence in 3 areas: hardware, software and applications.

In the area of computer hardware there is a need to re-do the original recommendations of the Task Force on Hardware for Real-Time Computer Laboratory Applications. Technology has advanced so rapidly that the original recommendations are completely out of date and are even misleading for many applications. It is also necessary to update the hardware descriptions to include some discussion of microprocessors which were not included in the original survey. Some of these particular developments are discussed in the CACHE Real-Time Task Force Note on Microprocessor Activities.

In the area of software there has been considerable progress in the provision of real time operating systems by minicomputer vendors. Most vendors now provide real time disk based operating systems which will handle multi-tasking program applications. These operating systems also support high level languages, such as FORTRAN and BASIC, as opposed to the original systems which were less sophisticated in this area. There has been a considerable input from the ISA and the Purdue Workshops on real time FORTRAN to the minicomputer vendors to the point where most vendors provide

the standard real-time FORTRAN subroutine calls which are being recommended. BASIC, as a language, is finding increasing use both from the teaching point of view and also for many industrial applications because of the ease of programming for new users, particularly undergraduates. Many industrial real-time applications are also written in BASIC or near BASIC language. Minicomputer systems and also microprocessor systems now make wide use of cassette tape operating systems and more recently floppy disk operating systems. The Task Force will address the problem of cassette systems as compared with floppy disk systems in the near future. These new moderate speed bulk storage devices make it possible for users with limited finances to be able to run the higher level languages which make the use of real-time computing in undergraduate laboratories and classes feasible.

In the area of applications of real-time computing the Task Force sees a strong need to provide descriptions and write-ups for experiments which make use of real time computing facilities. Originally some prototype experiments were provided but it has been realized since that what is needed is a series of ideas for experiments as opposed to detailed designs. Most academic users are interested in applying the real-time computer to their existing experiments or modified experiments as opposed to redesigning or rebuilding equipment to meet the particular design. In assessing the needs for applications, particularly at the undergraduate level, it is important to separate the concepts of data acquisition from those of control. Many typical undergraduate unit operations experiments could benefit very highly from the use of real-time computer equipment for data acquisition so that students could perform mass and energy balances on their experiments while they operate in a laboratory. Many of these applications do not require control.

Finally, the Real-Time Task Force is continually monitoring and assessing the need for short courses and conference sessions on both minicomputers and microprocessors. We are maintaining a close liaison with the minicomputer and microprocessor group involved with the 1977 Joint Automatic Control Conference, and also with the AIChE Machine Computation Committee which has expressed some interest in short courses at the AIChE Meetings.

## **CACHE REAL-TIME TASK FORCE ACTIVITIES ON MICROPROCESSORS**

The CACHE Real-Time Task Force originally published some recommended specifications on various minicomputer hardware configurations for chemical engineering laboratory data acquisition and control applications. With the rapid advances in technology these recommendations are very much out of date. In particular, with development of the microprocessors and microcomputer systems there is need to update the hardware discussion to include these new systems. Many new analytical instruments are being designed around microprocessors. Digital controllers and small one or two variable data acquisition systems are available. Distributed computing is now feasible in the laboratory environment. The Real-Time Task Force is going to address the problem of how the non-computer expert should exploit and make use of the

rapidly advancing technology in microprocessors.

In the undergraduate laboratory there is great scope for automation of lab experiments. The particular emphasis of improved experimentation is not to remove the students completely from the apparatus, but rather to develop the analytical power to provide on-line data reduction from experimentation. As a result, it should be possible to design experiments where the student explores the effects of many more variables or levels of operating conditions in the process. At the same time he is relieved of much of the tediousness of reduction of large amounts of laboratory data by hand or even by calculator.

Some of the major problems involved in using microprocessors are that although the microprocessor or microcomputer system itself is very inexpensive, software for these systems is virtually non-existent. If it is, it is often necessary to spend in the order of \$10,000 to \$15,000 for the vendor's operating system which often operates off a floppy disk or equivalent. It is necessary to explore the use of cross-compilers and cross-assemblers which could be run on either local minicomputer systems or on the large central computer facilities. Downloading of final versions of programs for testing from these higher level systems is necessary.

In the area of applications in the laboratory it is the intention of the Real-Time Task Force to try and provide the series of descriptions and write-ups for experiments. These would be written in such a way as to provide ideas as opposed to designs. It is important in these applications notes to separate the concepts, for example, those of data acquisition from control. Most chemical engineering users of minicomputer systems and probably microprocessor systems are more interested in general applications than in specific details of a particular experiment. On the other hand it is necessary to provide very explicit information on such apparently simple tasks as interfacing a thermocouple to the computer system. The same problems as are faced with minicomputer applications obviously follow for microprocessors. Technological developments in microprocessors now are such that many vendors are offering complete data acquisition modules which accept process measurements from standard transducers almost directly. There is a need to address the problem of the information gap between vendors and low level expertise users in this area.

## ASEE SUMMER SCHOOL

As part of the 1977 ASEE Summer Program for ChE Faculty, a program on Interactive Computing for Chemical Engineering Education will be conducted on Wednesday (AM and PM) and Thursday (AM only). The program will encompass computer graphics and technical information and data retrieval. The workshop co-leaders are: Prof. H. Scott Fogler, University of Michigan; Prof. Richard S. H. Mah, Northwestern University; and Prof. Brice Carnahan, University of Michigan.

The aim of this program is to develop an awareness in the chemical engineering community of the power and potential of interactive computing. Interactive computer graphics and technical information/data retrieval offer almost limitless possibilities for the development of instructional games and

simulation programs. Until recently these tantalizing possibilities have been beyond the reach of most educators because of computing and equipment costs. In the last few years the technology and economics have changed to make widespread application reasonable. Remote-access terminals will be available for workshop participants to use in practicing the techniques described in the lectures.

The following speakers (listed alphabetically) will participate in the program: Prof. R. P. Andres, Princeton; Prof. Bishop, Texas; Prof. B. Carnahan, Michigan; Prof. J. DiSalvo, Indiana; Prof. C. A. Eckert, Illinois; Prof. H. S. Fogler, Michigan; Dr. Kaufman, Manlabs; Prof. R. S. H. Mah, Northwestern; Prof. D. Rummer, Kansas; Prof. S. Smith, Illinois.

## FLOWTRAN PROCESS SIMULATION PROGRAM

In 1974, the FLOWTRAN process simulation program of Monsanto Company became available through CACHE for use by universities. Since then, annual workshops have been held to instruct professors in its use. In addition, a textbook entitled *FLOWTRAN Simulation—An Introduction* is available. The program is accessed by remote batch or remote job entry via a computer network. During fiscal year 1975-1976, FLOWTRAN was used by 34 chemical engineering schools. This compares to 25 user schools during fiscal year 1974-1975.

Recent developments in the CACHE FLOWTRAN project include:

1. **FLOWTRAN ARTICLE:** A brief article entitled "Use of FLOWTRAN Simulation in Education" and describing the history of the FLOWTRAN project in universities recently appeared in the Spring 1976 issue of *Chemical Engineering Education* (pages 90-92). Current and (especially) prospective FLOWTRAN users may find this description of how to access FLOWTRAN, how it is used, its extent of usage and future developments interesting and informative.
2. **PROBLEMS MANUAL:** A draft of a manual of FLOWTRAN demonstration problems for instructional purposes is currently being prepared by Professor J. Peter Clark of VPI&SU. There will be a total of 20-25 such problems in this manual.
3. **SEMINAR PRESENTATIONS:** New schools using FLOWTRAN and other schools thinking of using FLOWTRAN have found a useful seminar topic to be FLOWTRAN usage in process design, particularly since the FLOWTRAN Workshops are now being offered only once a year (next Workshop is scheduled for July 13-16, 1977 at the University of Wisconsin. For additional information, contact Mr. Hal Abramson at AIChE, 345 E. 47th St., N.Y., N.Y. 10017). Members of the FLOWTRAN Users Group are more than willing to make such seminar presentations. Persons interested in arranging such a seminar should contact one of the following regional FLOWTRAN representatives:

New England: NJ, PA, MD, DE, NY  
Warren D. Seider  
Department of Chemical Engineering  
University of Pennsylvania  
Philadelphia, PA 19174  
Southeast: NC, TN, SC, GA, FL, AL, MS  
Jude T. Sommerfeld

## UNDERGRADUATE LABORATORIES GIVEN ATTENTION

CACHE has established a new committee to look into opportunities to modernize the undergraduate laboratory using new technological developments. The committee co-chairmen are Scott Fogler (University of Michigan) and Grant Fisher (University of Alberta). Other committee members are Warren Seider (University of Pennsylvania), Joe Wright (McMaster), and Rudy Motard (University of Houston). Additional members are desired. Anyone wishing to serve as a committee member or to participate in some other capacity should contact Scott Fogler or Grant Fisher.

## COMING EVENTS

**PACHEC 77** (Second Pacific Area Chemical Engineering Conference), Denver, August 28-29, Host: AIChE.  
Computing with 1980s (2 sessions). Session co-chairmen: M. T. Tayyabkhan and T. I. Peterson  
Applied Numerical Methods. Session co-chairmen: B. Carnahan and L. Lapidus  
Simulation and Process Control in Pulp and Paper Production. Session co-chairmen: L. L. Edwards and T. J. Boyle

**New York AIChE Meeting**, November 13-17, 1977  
Computer Simulation Methods for Physical Properties (2 sessions). Session developers: Roy L. McCollough and Keith E. Gubbins  
Advances in Chemical Engineering Computing (2 sessions). Session developers: R. L. Motard and I. Rinard  
Computer Aided Resource Management. Session developer: R. E. C. Weaver  
Applied Mathematics and Information Processing in Electrochemical Systems. Session developers: J. R. Selman and D. Gidasporo  
New Design Methods in Control and Instrumentation. Session developer: W. Luyben

### Other Meetings

National Computer Conference, Dallas, June 13-16, 1977  
1977 Joint Automatic Control Conference, San Francisco, June 22-24, 1977

### Short Courses

New Developments in Modeling, Simulation, and Optimization of Chemical Processes, July 18-27, 1977, Massachusetts Institute of Technology. Contact Director of the Summer Session, MIT, Room E19-356, Cambridge, Massachusetts 02139.  
FLOWTRAN Workshop, July 13-16, 1977, University of Wisconsin, Madison, Wisconsin. Contact Mr. Hal Abramson, AIChE, 345 E. 47th Street, New York, N.Y. 10017  
Computer-Aided Design of Chemical Processes, July 11-15, 1977, Northwestern University. Contact Director, Continuing Engineering Studies, 2804 Technological Institute, Northwestern University, Evanston, Illinois 60201.