CACHE NEWS

News About Computers In Chemical Engineering Education.

No. 2

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PURPOSE OF THE CACHE COMMITTEE

The CACHE (Computer Aids for Chemical Engineering Education) Committee was established by the National Academy of Engineering's Commission on Education to accelerate and coordinate the introduction of digital computation in chemical engineering education. Members of the committee are all chemical engineering educators drawn from the faculties of U.S. and Canadian universities.

MEMBERS OF THE CACHE COMMITTEE

COMMUNICATION WITH THE CACHE COMMITTEE

The committee actively solicits the participation by interested individuals in the work of on-going CACHE projects. Anyone who wishes to learn more about current CACHE activities may contact any member of the committee or notify Mrs. Jean P. Moore, Commission on Education, National Academy of Engineering, 2101 Constitution Avenue, N.W., Washington, D.C. 20418 (Telephone 202—961-1417).

The CACHE Newsletter is published several times a year to report news of CACHE Committee activities and other noteworthy developments of interest to chemical engineering educators concerned with digital computation. Persons who wish to be placed on the mailing list should notify Mrs. Jean P. Moore at the address listed above.

Material for publication in the Newsletter is solicited from all sources. Submissions should be directed to the editor, Prof. Lawrence B. Evans, Room 12-111, M.I.T., Cambridge, Mass. 02139 (Telephone 617-864-6900 ext. 4580 or 4561).

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ABOUT THIS NEWSLETTER

This second edition of *CACHE News* is being sent to all chemical engineering department heads in the United States and to others who have asked that their names be placed on the CACHE mailing list. A reply form is provided on the last page of this newsletter for adding the names of anyone else who wishes to receive future editions of *CACHE News*.

The first issue of *CACHE News* was sent to all chemical engineering faculty members in the United States and Canada. About 350 of the approximately 2000 faculty members have written to ask that they receive future issues.

SECOND FORMAL MEETING OF CACHE COMMITTEE HELD IN SEPTEMBER

The second official meeting of the full CACHE Committee was held at Buck Hill Falls, Pennsylvania on September 2 and 3, 1971. The members of the committee had been working together on various subcommittee projects since the previous meeting in Ann Arbor, Michigan in April. The major activities at the second meeting involved receiving and approving reports of the subcommittees and planning further work.

An important decision reached at the meeting was to adopt a task force structure as a mechanism for carrying out CACHE Committee projects. The members of the task forces would include large numbers of people in addition to the CACHE Committee members and would involve people from industry and government as well as universities. When the task had been completed and the results of the work accepted and approved by the full CACHE Committee, the task force would be dissolved.

Several new task forces were established at the meeting to work on problems of estimation and retrieval of physical properties, making industrially developed systems for computer-aided design available for use at universities, and development of real-time systems for on line monitoring and control of chemical engineering experiments. Several of the existing subcommittee projects were redefined as task forces. The activities of each task force are described in separate articles in this newsletter.

GUIDELINES ADOPTED FOR SMALL PROGRAMS

A Subcommittee on Standards, with Professor Paul T. Shannon of Dartmouth as Chairman, has been grappling with the problem of establishing guidelines to facilitate inter-university interchange of computer programs and systems. As their initial activity, the subcommittee has focused upon establishing guidelines for programming, documenting, and testing small and medium size FORTRAN computer programs or subroutines of the type which are useful in classroom instruction. A document specifying these guidelines was approved by the full CACHE Committee at its meeting in Buck Hill Falls, Pennsylvania in September. They will apply to any computer program accepted by CACHE for publication or distribution.

The guidelines will be published eventually and be available from the CACHE Committee. Briefly, however, the guidelines specify that all FORTRAN programs must be written according to the USA Standard version of FORTRAN. Restrictions are also placed upon allowable program structure and size, the magnitude of constants, hardware requirements, communication with subroutines, and allowable input-output operations. Guidelines are set for general programming practice. Methods for documentation, especially applicable to programs intended for use in education, are specified. Procedures for testing programs are also outlined.

The first major application of the new guidelines will be to programs accepted for publication by the CACHE Cur-

riculum Subcommittee in its six-volume collection of computer programs used in undergraduate courses. Meanwhile, the Standards Subcommittee is considering other areas in which guidelines are needed, including programs written in specialized languages for dynamic system simulation such as CSMP (Continuous System Modeling Program) and large process simulation systems. A paper summarizing the developments in the standards area will be presented by Professor Shannon at the St. Louis meeting of the AIChE in May, 1972. Additional members of the Standards group are Professors Grens, Hughes and Klaus.

SEADER TO HEAD TASK FORCE ON LARGE SYSTEMS

Professor J. D. Seader, of the University of Utah, has been named to head a CACHE task force which will investigate the feasibility of making available to universities some of the large-scale computer programs developed by industry for computer-aided chemical process design. Until about the middle 1960's computer-aided process design was almost the exclusive province of several universities and a few companies which could afford large computing facilities and which had the necessary process design and programming talent. In recent years, however, a number of comprehensive process design systems have been developed by industry. Some of these, such as CAPS, FLOWTRAN, PACER 245, PDA, and others are available commercially for sale or lease. Other proprietary systems are used only within the company which developed them; this appears to be the situation with such companies as duPont, Esso, and Shell.

Professor Seader commented, "Unfortunately, university education in computer-aided process design now appears to be lagging behind industrial practice. This situation has arisen despite efforts to make early versions of programs like PACER 1.0 and CHESS available to any chemical engineering department at a nominal cost. One reason for this is because the implementation of such large programs at a local university computing center requires educators who possess both design and programming experience as well as a willingness to spend considerable time first in modifying the program to make it function properly on the particular computer and then in maintaining it."

Professor Seader's task force is investigating the feasibility of making some of the large proprietary programs developed by industry available to universities. One approach would be to maintain the large programs on a central computing facility which could be accessed at individual universities from remote batch or teletype terminals communicating over telephone lines. This would relieve individual professors of the responsibility for maintaining large systems, but would introduce a problem in paying the cost of communications and computing facilities.

One question which the task force must face is that of deciding under what conditions an industrially developed program would be appropriate for university use. Does one, for example, need to have access to the source programs of these large systems in order to be able to use them effectively? Or, can the programs be treated as black boxes and used with limited knowledge of their internal workings? Another question: are these large programs too complicated and require too much computer time to solve classroom problems which emphasize concepts?

From the viewpoint of industry, it is not at all clear whether companies would be interested or willing to make their proprietary programs available to universities. The terms under which they would be willing to let students use their programs would have to be worked out to insure that proprietary interests are not compromised. Some of the benefits to industry from making the systems available for use in education include the availability of better-educated engineering graduates, development of a market for the programs, and the assistance of universities in preparing teaching materials to facilitate use of the programs. The first step has been to send a letter to all major companies known to have a computer-aided process design program. Once the status and availability of the programs is known, then the task force can begin addressing some of the more difficult questions of making them available on a feasible basis.

There is some precedent for letting universities use industrially developed programs. In the mid-1960's, the Chevron Research Company made its generalized heat and material balancing system available to a limited number of academic institutions for use in teaching and research. The system was operational at the University of California (Berkeley) and copies of the program were provided to the University of Michigan and to M.I.T. Digital Systems implemented PACER 245 at Cornell University last year, and PACER was used in teaching and research. More recently, Dr. William Svrcek at the University of Western Ontario has become a FLOWTRAN customer and plans to use the service in teaching. He signed the regular agreement and will be paying the same rates as any commercial FLOWTRAN customer.

The task force welcomes input from interested individuals from both universities and industry. The experience of anyone who has used large industrial systems for education would be particularly welcome. Comments should be directed to Professor Seader at the University of Utah.

PUBLICATION OF CLASSROOM CUMPUTER PROGRAMS IS PROCEEDING ON DELAYED SCHEDULE

The curriculum subcommittee of CACHE received an overwhelming response to the letter sent to each chemical engineering faculty member on April 30, inviting them to submit programs which had been used successfully in the classroom. About 500 abstracts were received. On the basis of the abstracts, it appeared that the quality of most of the programs is excellent. Responses were received from all over the world, including entries submitted from Taiwan, Japan, Africa, and Australia, in addition to the numerous responses from South America and Europe.

Most of those who submitted abstracts have been asked to supply additional information to clarify the nature and

method of use of their programs. All of the authors are being notified to indicate whether or not their problems have been accepted for publication.

Professor Ernest Henley of the University of Houston, Chairman of the Curriculum Subcommittee, stated, "We apologize for the long time lapse between abstract submission and program acceptance. Because of the large number of programs submitted, the selection, budgeting, and determination of a publication procedure proved to be more time-consuming than we had anticipated." The subcommittee hopes to publish the six-volume set of books early in 1972. This will require that all authors send their contributions by the end of February and that minimal delays are encountered at the publisher.

TASK FORCE ESTABLISHED FOR REAL-TIME COMPUTING

An excellent response was received from a survey "Of the Nature and Extent of Real-Time Computing at Colleges and Universities in the United States and Canada". A letter was sent by Professor Lawrence Evans, Chairman of the New Projects Subcommittee of CACHE, to all chemical engineering department heads in these countries in May, 1971. Replies were received from eighty-three of the 153 universities contacted. Of these, twenty-nine had some real-time equipment in use for on line monitoring and control of chemical process apparatus. An additional nineteen universities were planning to get such equipment in the near future, and twenty-one offered some sort of instruction to their students in this area.

Because of the wide interest in the field, the CACHE Committee has established a task force to determine what work is needed to coordinate and encourage the appropriate use of real-time computing in the chemical engineering curriculum. Professor Eugene Elzy of Oregon State University is heading the task force and additional members include Professors Lawrence Evans (M.I.T.), Duncan Mellichamp (University of California at Santa Barbara), Roger Schmitz (Illinois), Dale Seborg (Alberta), Cecil Smith (L.S.U.), Robert Weaver (Tulane), Arthur Westerberg (Florida), Theodore Williams (Purdue) and Joseph Wright (McMaster). Members from industry are Thomas Gaspar (Merck) and John Ornea (Shell Development).

Professor Elzy noted, "The objectives of the task force are to assess the role of real-time systems in the curriculum and to prepare a report by December, 1972 including course outlines and/or curriculum guides using real-time systems, three or four prototype systems as examples along with complete equipment lists, costs, and a guide to available hardware and software for on-line computer systems." The first meeting of the task force will be held at the San Francisco meeting of the AIChE this year.

PROPERTIES TASK FORCE FORMED

The CACHE committee has formally established a task force, chaired by Professor R. L. Motard of the University of Houston, to consider methods for integrating computer-based methods for estimation and retrieval of physical properties into the chemical engineering curriculum. Members of the task force from universities include Professors Frank Canfield (Oklahoma University), Ronald Klaus (University of Pennsylvania), John O'Connell (University of Florida), Michael Samuels (University of Delaware), Warren Seider (University of Pennsylvania), and Grant Wilson (Brigham Young University). Members of the task force from industry include Bob Cavett (Monsanto), Ted Leininger (DuPont), and Ted Stein (Halcon). Dr. Newman Hall (Commission on Education) is also a member. All of the task force members have been actively involved in the development and use of methods and computer programs for physical property determination.

The task force held its first meeting during the summer in Atlanta. After first reviewing the current status of the use of physical property data, the task force identified two major areas where work was needed: the preparation of new curriculum material and the development of more usable computer systems for property calculations. The task force divided itself into two subgroups to work in each of these areas.

The first subgroup (Motard, Cavett, Samuels, Wilson, O'Connell, Seider, and Stein), dealing with curriculum, plans to prepare a comprehensive workbook or report to serve as a curriculum guide on the use of physical properties in the undergraduate program. The curriculum guide will contain sections dealing with sources of physical property data, uses of data, estimation techniques, sensitivity of process calculations to the accuracy of data or estimation methods, and examples of small design projects with a strong dependence on properties. The subgroup hopes to complete a report in time for presentation at the ASEE Summer School in Boulder, Colorado in August, 1972.

The second subgroup (Klaus, Leininger, Canfield, Motard, and Stein) will focus upon the problems of developing information systems from a software point of view. Their initial product will be the design of a computer-based physical properties system which will include specifications for an overall system structure, description of data structures and techniques for data communication, algorithm structures, interfaces with operating systems, methods of extracting small subsets of the complete system for specialized applications, and the interface to design and simulation programs. The subgroup hopes to complete a preliminary draft of a report containing their results by the end of 1971.

RESULTS TABULATED FROM SURVEY ON DYNAMIC SYSTEMS

Results have been tabulated from an informal survey conducted by the CACHE Subcommittee on Dynamic Systems and Control. A questionnaire was mailed to chemical engineering department heads in the United States and Canada in June to determine the interest and level of use of dynamic system simulation in the undergraduate and graduate curriculum.

There have been fifty-six respondents to the survey. Some brief statistics follow: 70% indicated the digital computer was being used in teaching process dynamics and control. 36% are using the computer in other courses such as design and analysis in addition to the control course usage. The latter are principally elective courses whereas most of the process dynamics and control courses are listed as required.

The Dynamic Systems and Control Subcommittee has organized a seminar on "The Role of the Computer in Teaching Undergraduate Process Dynamics and Control", scheduled for Wednesday afternoon, December 1 (from 4:30 to 6:30 p.m. in the Olympic Suite of the St. Francis Hotel) during the Annual AIChE meeting in San Francisco. A primary purpose of the seminar will be to seek discussion from participants, both academic and industrial, concerning the role of dynamic systems simulators in the undergraduate program.

SYMPOSIUM ON COMPUTER-AIDED PROCESS SYNTHESIS SET FOR DALLAS AIChE MEETING

A two-part symposium entitled "Computer-aided Process Synthesis" has been finalized for the 71st National Meeting of the AIChE to be held in Dallas, Texas, February 20–23, 1972. Co-chairmen for the symposium are CACHE Committee Members Professor J. D. Seader of the University of Utah and Professor Eugene Elzy of Oregon State University.

Many of the researchers working in this relatively new area of chemical engineering will be on hand to present results of their studies. The program will consist of the following papers:

1. R. W. Thompson and C. J. King:
   "Systematic Synthesis of Separation Schemes"
2. G. J. Powers and D. F. Rudd:
   "Heuristic Synthesis in Process Development"
3. M. A. Menzies and A. I. Johnson:
   "Synthesis of Optimal Energy Recovery Networks using Discrete Methods"
4. J. Hendry and R. R. Hughes:
   "The Synthesis of Optimal Separation Sequences by List Processing Techniques"
5. A. Ichikawa and L. T. Fan:
   "Necessary Condition for Optimal Process Techniques"
6. R. L. McGalliard and A. W. Westerberg:
   "Structural Sensitivity Analysis in Design Synthesis"
7. T. Umeda and A. Ichikawa:
   "Synthesis of Optimal Processing System by a Method of Decomposition"
8. D. J. Wilde:
   "Differential Optimization of Structured Systems"
9. R. W. Neumann and J. H. Hamlett:
   "Dynamic Process Simulation for Plant Design using Digital Computers"

Anyone interested in chemical-process synthesis is invited to attend the two sessions at Dallas and enter into the discussions on the papers. Dr. Seader and Dr. Elzy may be contacted for further information.

LOCAL CACHE REPRESENTATIVES DESIGNATED

A letter has been sent from Professor Warren D. Seider, Chairman of CACHE, to a specific faculty member at each of the 153 United States and Canadian chemical engineering departments, formally inviting them to serve as the official representative of their institution for liaison with the CACHE Committee. The names of the local representatives who have agreed to serve will be published in the next issue of *CACHE News*. The primary function of the local representative to CACHE will be to serve as a focal point for communication between the CACHE Committee and his institution.

COMPUTER-BASED AIR POLLUTION GAME BEING DEVELOPED

A computer-based air pollution game which may be used to aid a variety of undergraduate programs in colleges and universities around the United States is being designed at Carnegie-Mellon University under a $25,000 grant from the Esso Education Foundation.

Heading the project is Matthew J. Reilly, associate professor of chemical engineering and member of the CACHE Committee. Assisting are Anthony S. Walters, assistant dean of the School of Urban and Public Affairs, and a team of undergraduate students.

The game, which is expected to be developed by the end of the year and made available to schools around the nation, will be applicable to undergraduate courses dealing with environmental problems. Students from many disciplines—engineering, economics, urban studies, and other—will be able to use the game to solve simulated air pollution problems. The game will serve as a supplement to classroom instruction and visits by professionals from air pollution control agencies and related industries.

According to Dr. Reilly, the game will enable students to learn more about the complexities of air pollution problems and become better equipped to deal with them.

"After grappling with the complexities of a simulated air pollution problem and devising a satisfactory solution," he says "students will be much better prepared to tackle a real problem and learn from industrial and regulatory personnel."

He points out that students need to learn that solutions to complex environmental problems are attainable but require expert planning, organization and analysis, and that air pollution problems involve technology, health, law, economics, and the resolution of conflicts among sections with diverse values, interests and aims.

"But," he notes, "the traditional classroom lecture must be augmented if we are to meet these instructional objectives. The air pollution game is one way of doing so."

Students, who will assume roles as members of air pollution boards, emission sources, and citizen groups, will play

the game by first designing an alert warning system for the avoidance of acute air pollution "episodes." When confronted with a set of adverse meterological conditions simulated by the computer, the players will activate the alert system. The computer will report the resulting air quality with associated costs and benefits, and the students will evaluate the strengths and weakness of the simulated performance. Faculty members and pollution control members will assess the performance also.

Development of the game, Dr. Reilly says, is being carried out with the aid of undergraduate students, who test and modify preliminary versions. He adds that the game is a forerunner of the types of innovations expected to come out of Carnegie-Mellon's Environmental Studies Institute.

Funding for the air pollution project is a part of a total $100,000 award by Esso to four major universities for the improvement of undergraduate education in the United States. Also receiving $25,000 each were Harvard University, Massachusetts Institute of Technology, and George Washington University.

CALENDAR OF EVENTS

The Calendar of Events is a regular feature of the CACHE *News*. It lists meetings, symposia, workshops, special courses, and other events of interest to chemical engineering educators concerned with the use of computers. Please notify the editor of events to be included in future issues.

Activities officially sponsored by the CACHE Committee are noted with an asterisk (*). The person to contact for further information about any event is indicated in parenthesis.

November 28–December 2, 1971 AIChE 64th Annual Meeting, San Francisco

Symposium on Advances in Chemical Engineering Computing (T. I. Peterson, IBM Cambridge Scientific Center, 545 Technology Square, Cambridge, Massachusetts 02139).

*Seminar on Dynamic Systems and Control in the Undergraduate Chemical Engineering Program, Wednesday, December 1, 4:30–6:30 P.M. in the Olympic Suite of the St. Francis Hotel. (A. I. Johnson, Dean, Faculty of Engineering Science, University of Western Ontario, London, Ontario, Canada).

February 20–23, 1972 AIChE 71st National Meeting, Dallas

Symposium on Computer-Aided Design (C. M. Qualline, Systematic Design, Inc. 2702 National Drive, Garland, Texas 75040).

Symposium on Optimization Techniques (R. W. Pike, Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803).

Symposium on Use of Computers in the Educational Process (J. J. Lagowski, Department of Chemistry, University of Texas, Austin, Texas 78712).

*Symposium on Computer-Aided Process Synthesis (J. D. Seader, Department of Chemical Engineering, University of Utah, Salt Lake City, Utah 84112).

May 21–24, 1972 AIChE 72nd National Meeting, St. Louis

*Symposium on CACHE Update—Computer-Aided Chemical Engineering Education (W. D. Seider, School of Chemical Engineering, 375 Towne Building, University of Pennsylvania, Philadelphia, Pennsylvania 15213).

Symposium on Plant Applications of Computers (C. W. DiBella, Monsanto Company, 800 North Lindberg Boulevard, St. Louis, Missouri 63166).

Symposium on Advances in Process Optimization (V. J. Law, Department of Chemical Engineering, Tulane University, New Orleans, Louisiana 70118).

Symposium on Computer Methods in Process Design, (C. H. Chien, Monsanto Company, 800 North Lindberg Boulevard, St. Louis, Missouri 63166).

June 19–30, 1972 Special Summer Program on "New Developments in Modeling, Simulation, and Optimization of Chemical Processes," Massachusetts Institute of Technology, Cambridge, Massachusetts 02139. (Professor L. B. Evans, telephone 617-864-6900 x 4580 or 4561).

August 13–18, 1972, ASEE Summer School for Chemical Engineering Faculty, Boulder, Colorado. (Director, L. Bryce Andersen, Newark College of Engineering).

Workshop on Chemical Process Design and Engineering. (C. J. King, E. Grens, A. Foss, and S. Lynn, University of California, Berkeley; D. Rudd, University of Wisconsin).

Workshop on Integration of Biomedical and Environmental Applications of Chemical Engineering into Undergraduate Courses (R. Seagrave, Iowa State University; Giles Cokelet, Montana State University).

Workshop on Application of Molecular Concepts for Predicting Properties Needed for Design (J. O'Connell and K. Gubbins, University of Florida; J. Prausnitz, University of California at Berkeley).

Workshop on Numerical Methods for Chemical Engineering Problems (J. O. Wilkes and B. Carnahan, University of Michigan).

Workshop on New Developments in Undergraduate Laboratories (A. Perna, Newark College of Engineering; S. Fogler, University of Michigan; F. Shair, California Institute of Technology).

Two afternoon sessions will be devoted to a presentation of recent CACHE Committee activities. (R. V. Jelinek, on leave from Syracuse University, E. J. Henley, University of Houston, and E. Grens, University of California at Berkeley).

August 27–30, 1972 AIChE 73rd National Meeting, Minneapolis

Symposium on Applied Numerical Methods (M. R. Samuels, Department of Chemical Engineering, University of Delaware, Newark, Delaware 19711).

November 26–30, 1972 AIChE 65th Annual Meeting, New York City.

Symposium on Advances in Chemical Engineering Computing (M. T. Tayyabkhan, Mobil Research and

Development Company, P.O. Box 1026, Princeton, New Jersey 08540).

October 23-27, 1972 International Symposium on Systems Engineering and Analysis, Purdue University, Lafayette, Indiana (Professor G. V. Reklaitis, School of Chemical Engineering, Purdue University, Lafayette, Indiana 47907).

March 11-15, 1973 AIChE 74th National Meeting, New Orleans

Symposium on Optimization Theory and Applications (R. W. Pike, Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803).

Please place the following names on the mailing list to receive future issues of *CACHE News*.

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