CACHE NEWS

News About Computers In Chemical Engineering Education.

No. 3

March, 1973



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

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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 News is published one or two 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 CACHE News is solicited from all sources. Submissions should be directed to the editor, Prof. Lawrence B. Evans, Room 12-135, M.I.T., Cambridge, Mass. 02139 (Telephone 617-253-4580).

The work of the CACHE Committee is supported in part by the National Science Foundation under Contract C310, T.O. 196.

CONTENTS

Section of the second section of the section of the second section of the section of the second section of the sectio	
	Page
ABOUT THIS NEWSLETTER	1
FIRST TWO VOLUMES OF CACHE	
COMPUTER PROGRAMS PUBLISHED	1
CACHE MEETS TO PLAN PROJECTS AND	
ELECT OFFICERS AND NEW MEMBERS	1
CHRISTENSEN TO HEAD TASK FORCE ON	
MODULAR INSTRUCTION	2
SEIDER TO HEAD TASK FORCE ON	
PROGRAM DISTRIBUTION	2
PROPERTIES TASK FORCE PUBLISHED	
REPORT	3
CACHE PROPOSES GUIDELINES FOR	
LARGE-SCALE COMPUTER PROGRAMS	3
WORKSHOP PROMOTES USE OF DIGITAL	
COMPUTER FOR DYNAMIC	
SIMULATION	3
SYMPOSIUM ON PROCESS SYNTHESIS	
STIMULATES NEW WORK	4
TASK FORCE PROMOTES REAL-TIME	
COMPUTING IN THE LABORATORY	4
FORRESTER MODEL OF WORLD	
DYNAMICS AVAILABLE IN FORTRAN	4
UNIVERSITY OF COLORADO ChE's BUILD	
COMPUTER SYSTEM	4
UCSB DEVELOPS REAL-TIME COMPUTING	
FACILITY	5
CACHE COMMITTEE FUNDED BY NSF FOR	
ADDITIONAL THREE YEARS	5
CALENDAR OF EVENTS	5
LOCAL CACHE REPRESENTATIVES	
DESIGNATED	6
DEGRAM THE STATE OF THE PROPERTY OF	trail.
TO BE PLACED ON CACHE MAILING LIST	7
Charles and the charles and th	

ABOUT THIS NEWSLETTER

This third edition of CACHE News is being sent to all local CACHE representatives and to any 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 previous issue of CACHE News appeared in November, 1971. We expect that future editions will be published about once or twice each year.

FIRST TWO VOLUMES OF CACHE COMPUTER PROGRAMS PUBLISHED

The first two volumes of the seven-volume set of computer programs for chemical engineering have been mailed out to all departments of chemical engineering. These are *Stoichiometry*, edited by E. J. Henley of the University of Houston, and *Kinetics* edited by Professor Matthew J. Reilly of Carnegie-Mellon University. The preliminary reaction of individuals who have seen the book is that they will be a valuable aid to chemical engineering educators interested in using the computer in each of these areas.

Additional copies of these books may be obtained by writing Professor E. J. Henley, Chemical Engineering Department, University of Houston, Houston, Texas 77004. Volume I, Stoichiometry, contains 13 programs is 228 pages long, and costs \$4.00. Volume II, Kinetics, contains 21 programs, is 380 pages long, and is available for \$4.50.

CACHE MEETS TO PLAN PROJECTS AND ELECT OFFICERS AND NEW MEMBERS

In the year and a half since the last issue of CACHE News, there have been three meetings of the full CACHE Committee. The Committee met in December, 1971 at the Sonoma Valley in California; it met in May, 1972 at the Lake of the Ozarks in Missouri; and it met in December, 1972 at Grossinger, New York. The major function of the meetings has been to discuss and approve task force reports and plans for future work and to initiate new projects.

At the May, 1972 meeting, the present slate of officers consisting of Warren D. Seider as Chairman, Lawrence B. Evans as Vice-Chairman, and Arthur W. Westerberg as Secretary were re-elected for another year. In the future, new officers will be elected each Spring and the vice-chairman will automatically become chairman in the following year. Therefore, in May, 1973 Professor Evans will become chairman of the committee and a new vice-chairman and secretary will be elected.

At the December, 1972 meeting the committee elected three new members. They were Professor David M. Himmelblau (University of Texas), Professor Gary J. Powers (MIT), and Professor Cecil L. Smith (LSU). Members of the

committee serve for a three-year period. There will be seven additional openings in 1973 and 10 openings in 1974 as the committee evolves to staggered terms of service.

CHRISTENSEN TO HEAD TASK FORCE ON MODULAR INSTRUCTION

At its December, 1972 meeting, CACHE approved the establishment of a Task Force on Modular Instruction with Professor James H. Christensen of the University of Oklahoma as chairman.

Its purpose is to facilitate experimentation and flexibility in ChE curricula through widespread knowledge and practice of modular instruction. Under any of several names, e.g., the "Keller plan", this basically involves the splitting of traditional course content into many well-designed learning experiences. Each such module contains:

- A Statement of prerequisite skills and a "pre-test" to assure that the student is ready for the module;
- A statement of objectives, i.e., skills that the student is to acquire upon successful completion of the module;
- A set of materials necessary to provide a self-paced learning experience;
- A post-test designed to assure that the student possesses the skills stated in part (2);
- A resource document to help the teacher determine how and where the module may be used in his course.
 While modules may be used to supplement or supplant

traditional lectures, it is important to note that the emphasis throughout is on the student's experience and not the teacher's; thus, this is student-centered teaching!

One of the first jobs of the task force is to *identify* those who are currently using modular instruction in chemical engineering and to set up an informal *communications* network for sharing ideas, experiences, and maybe even modules. If you know anyone who is engaged in modular instruction, please have him drop a note to:

Professor James H. Christensen School of Chemical Engr. & Materials Sci. University of Oklahoma

202 W. Boyd, Room 23

Norman, Oklahoma 73069

with as much of the following information as possible:

Name and address

Course title and outline of module topics

Description of media used

Teacher and student reaction to the course

Suggestions for improvement

Individuals interested in joining the task force should also contact Professor Christensen.

SEIDER TO HEAD TASK FORCE ON PROGRAM DISTRIBUTION

A major concern of the CACHE Committee has been the dissemination of computer-based instructional materials to chemical engineering educators and students at remote locations across the country. At its December, 1972 meeting, CACHE formed a Program Distribution Task Force, chaired by Professor Warren D. Seider (University of Pennsylvania) for the purpose of establishing viable mechanisms for distributing computer programs and providing access to computing resources. Other members of the task force include Professors J. D. Seader (Utah), R. R. Hughes (Wisconsin), P. T. Shannon (Dartmouth), and L. B. Evans (MIT).

During the past year, the CACHE Committee has been following closely the development of communication networks that link computers together at different universities. Such networks enable all participating universities, some without computers of their own, to use any computer program installed on any of the network computers.

One notable example is the ARPA Network (ARPANET) established by the Advanced Research Projects Agency of the Department of Defense to facilitate research in networking technology. This network links over 30 computers together across the country. Users have access to the ARPANET for the price of a local phone call in cities where a network computer resides.

Other networks have been organized on a regional basis and are gaining in popularity. A few examples are TUCC (Triangle Universities Computing Center in North Carolina), NERCOMP (New England Regional Computing Program), and MERIT (Michigan Educational Research Information Triad). Others are under development in Pennsylvania, Illinois, Washington, California, Texas, and Iowa. Some commercial firms have also developed computer networks to supply remote batch and timesharing services nationwide. Examples include those of United Computing Systems, Inc. and the General Electric Company.

Since its inception in 1969, the CACHE Committee has sought a mechanism for distribution of large-scale programs for computer-aided analysis and design, estimation of physical properties, dynamic simulation and control studies, among others. While most of these programs have been developed in FORTRAN to allow for machine interchangeability, program maintenance has been a major obstacle to their widespread usage. Most departments of chemical engineering are not equipped to maintain a large program library.

In the summer of 1972 the CACHE Committee sponsored an experiment in which two typical computer programs were placed on the network. ARPA very generously provided access to the network to conduct the networking experiment. The programs were installed on a PDP/10 computer belonging to Bolt Beranek and Newman in Boston by Professor Ronald L. Klaus and Mr. Gregory Powers of the University of Pennsylvania. The first program was a comparatively simple program to simulate a nitric acid plant; the second program was the large and complicated Pennsylvania Physical Property Information System (PPPIS). The first of these programs was successfully demonstrated at the ASEE Summer School for chemical engineering professors held in Boulder, Colorado in August, 1972.

The National Science Foundation's Office of Computing Activities has proposed to establish a trial National Science Network over the next five-year period. The trial network is to be implemented on the basis of current computer communications technology and augmentation of selected computer-based resources for effective network utilization. The CACHE Program Distribution Task Force is actively exploring ways in which CACHE can participate in experiments to use the new National Science Network to distribute computer programs for use in chemical engineering education.

In its enthusiasm for national computing networks, the CACHE Program Distribution Task Force is not overlooking other methods of program distribution that have been quite successful for small-scale programs; e.g., cards and tapes. It is planned that all 125 programs that appear in the seven-volume set of programs for use in course work will be distributed on magnetic tape. Furthermore, many of the new program modules under development for individualized instruction will run on minicomputers and may be distributed using cassette tapes.

Professor Seider encourages anyone who is interested in serving on the Program Distribution Task Force to contact him at the Department of Chemical Engineering, 375 Towne Building, University of Pennsylvania, Philadelphia, Pennsylvania 19104.

PROPERTIES TASK FORCE PUBLISHES REPORT

A useful source document, the CACHE Physical Properties Data Book, was published in August, 1972 and has been sent to all chemical engineering departments. This report is the work of Dr. M. R. Samuels, formerly of the University of Delaware and now with the DuPont Company. The preparation of a second report, The Curriculum Guide on Physical Properties, is now being coordinated by Professor John P. O'Connell at the University of Florida.

A subgroup of the task force is working to produce specifications for a computer-based physical properties information system. The subgroup produced its first tentative report for the St. Louis Meeting of the A.I.Ch.E. in May, 1972. They are now in the process of refining the design of this software system for undergraduate use. New members recently added to the task force to work in this area are Prof James H. Porter of MIT and Dr. Norman Carnahan, of Rice University.

CACHE PROPOSES GUIDELINES FOR LARGE-SCALE COMPUTER PROGRAMS

In September, 1971, the CACHE Committee issued the document, Standards for CACHE FORTRAN Computer Programs. This document, which was revised in May, 1972, set forth preliminary working guidelines governing programming, documentation, testing, and distribution for approximately 100 FORTRAN computer programs that are currently being published in seven volumes for distribution

to chemical engineering departments and for sale to individual chemical engineering educators (see lead article in this newsletter).

In general, the May, 1972 guidelines apply to individual self-standing programs or subroutines that can be implemented readily by the user at his own computing center. The CACHE Committee has now completed a second document on guidelines which apply to large-scale or complex systems of programs that are best installed and maintained at one computer center with remote access provided for users elsewhere. Such systems are referred to as "large-scale systems." This new document has been distributed to all CACHE local departmental representatives. The CACHE Committee is now making plans to solicit large-scale programs from educators and industry.

It should be noted that the "Guidelines" document is a working document, subject to modification and improvement. Any suggested changes should be sent to Prof. J. D. Seader, Chairman of the Large Scale Systems Task Force, Dept. of Chemical Engineering, University of Utah, Salt Lake City, Utah, 84112.

WORKSHOP PROMOTES USE OF DIGITAL COMPUTER FOR DYNAMIC SIMULATION

A workshop on Dynamic Simulation and Control was held at Purdue University on October 26-28, 1972. This was sponsored by the Task Force on Dynamic Systems and Control. The objective was to promote the use of digital computer simulation as an effective aid to instruction in chemical engineering at both the undergraduate and the graduate level.

Roger Franks was the principal lecturer with assistance provided by John Woods. Mr. Franks gave a description of the construction and use of his DYFLQ, a library of thirty modular routines for modeling the dynamic behavior of continuous systems. Elementary modules are present for unit operations with and without holdup, controllers, and various control elements as well as service routines for describing the state of a stream and for solving non-linear algebraic and differential equations. These are documented thoroughly in Frank's new book, Modeling and Simulation in Chemical Engineering (Wiley, 1972). In contrast to simulation programs such as DYNSYS and REMUS, the user writes his own executive program for specifying the process topology and proper sequencing of calculations through a series of calls to the DYFLQ libraries.

In order to provide a working knowledge for using the system, the lecture material was supplemented with a number of short programming exercises leading to a dynamic model of a small process, complete with controllers. Workshop participants had the opportunity to run these problems or to operate an existing model of the process.

Two versions of the DYFL@ library have been assembled; one for large machines such as the CDC 6000 series and another for smaller machines such as the IBM 1130 and CDC 1700. An over-lay version to permit a form of user interaction is available on the CDC 1700. Copies of the

libraries may be obtained from Prof. J. M. Woods, School of Chemical Engineering, Purdue University, West Lafayette, Indiana 47907. The programs are available without charge except for postage and handling.

SYMPOSIUM ON PROCESS SYNTHESIS STIMULATES NEW WORK

A two-part symposium entitled "Computer-Aided Process Synthesis" was sponsored by the CACHE Committee and held at the 71st national meeting of the AIChE in Dallas, Texas on February 20-23, 1972. Co-chairmen for the symposium were CACHE Committee members Professor J. D. Seader of the University of Utah and Professor Eugene Elzy of Oregon State University. Over 100 persons attended the two sessions to listen to papers representing the most recent studies by workers in this relatively new area of process design research. Several algorithms of interest to both educators and industry are now available for conducting process synthesis. A review article on the subject appeared in the January, 1973 issue of the AIChE Journal.

TASK FORCE PROMOTES REAL-TIME COMPUTING IN THE LABORATORY

During the past year a CACHE task force headed by Professor Eugene Elzy of Oregon State University has been concerned with introducing real-time computers into the undergraduate chemical engineering curriculum.

The first objective of this task force is to teach students about minicomputers and real-time systems. Hands-on experience with real-time hardware, interfacing and instrumentation, and real-time programming experience are essential.

Improving the teaching of undergraduate process dynamics and control is a second objective. The third objective is to demonstrate advanced computer control techniques, including DDC (Direct Digital Control). Improving laboratory efficiency and student motivation by instant analysis of data and calculation of results—for example in the unit operations and transport phenomena laboratories, is the fourth objective.

To facilitate the introduction of real-time computers by chemical engineering faculty, the task force will initiate such projects as:

- ... a one-to-two-week workshop for faculty during the summer of 1974
- ... a collection of fully documented prototype experiments now being used in various chemical engineering departments
- ... a collection of course materials such as outlines and specially-prepared instructional modules
- ... guidance on the selection of real-time computing equipment

To aid in the selection of real-time computing equipment, a tentative proposal for specifications of a computer system for use in the chemical engineering curriculum has been prepared by the task force. The statement of specifications takes the form of a recommended full-size system and two subsets of it: a basic convenient-size system and a minimum-size system. The minimum system must be field expandable through the convenient-size to the full-size system. The proposed specifications should be a useful resource document for a department desiring to add real-time computing hardware. Although these specifications are presently under further evaluation by others outside the task force, copies are available.

Copies of the proposed real-time computer specifications, examples of real-time course outlines and further information pertaining to the activities of the real-time task force may be obtained by writing Professor Eugene Elzy, Department of Chemical Engineering, Oregon State University, Corvallis, Oregon 97331.

FORRESTER MODEL OF WORLD DYNAMICS AVAILABLE IN FORTRAN

The global computer model developed by Professor Jay W. Forrester of MIT which is detailed in his book "World Dynamics" (Wright-Allen Press, Inc., Cambridge, Massachusetts) has received widespread attention. The model gives long term projections of world population, pollution level, capital investment, depletion of natural resources and the "quality of life." Students are particularly interested in the model, both from a mechanistic point of view as an illustration of the power of mathematical modelling and simulation, and in terms of its economic, sociological and ecological implications.

The Forrester model has been programmed in FORTRAN IV and is now available from the Department of Chemical Engineering, Lehigh University. The program is provided as a source deck which is thoroughly documented with comment cards that define all variables and cross reference all equations to Forrester's book. Output from the program includes line printer plots which essentially duplicate the plots in Forrester's book, The program is available as a package consisting of a source deck (approximately 1500 cards in standard FORTRAN IV including the plotting routine, punched in the 026 character set), a listing of the program and a sample of the output for \$30.00 which covers the cost of preparation, testing and mailing (please make checks payable to Lehigh University and mail to W. E. Schiesser, Department of Chemical Engineering, Lehigh University, Bethlehem, Pennsylvania 18015).

UNIVERSITY OF COLORADO CH.E.'s BUILD COMPUTER SYSTEM

Working under a National Science Foundation grant of \$10,900, the Department of Chemical Engineering at the University of Colorado is building a data acquisition and control computer system for laboratory and research use.

The system is based on a Data General Nova 1210 minicomputer with 8K words of core memory, and its configuration includes 32 differential variable-gain analog inputs, 4 analog outputs, 16 relay-buffered digital inputs with optional interrupt on change of state, 16 relay buffered digital outputs, a numeric keyboard and digital display, and 16 illuminated push-button switches, plus the standard fare of ASR33 teletype and realtime clock.

Data General's BASIC language with realtime CALL extension will be the major software tool. A realtime operating system for general data acquisition use will also be developed.

By designing and building the interface system themselves, Colorado is realizing savings of more than \$6,000. The project and grant are supervised by W. Fred Ramirez, Department Chairman, and system design and construction are the responsibility of David E. Clough, a chemical engineering doctoral student. Details of the system are available from either of the above. Their design is complete and the system will be operational by the first of the year.

UCSB DEVELOPS REAL-TIME COMPUTING FACILITY

A NOVA (Data General) computer with 20K core memory and a 256K fixed-head magnetic disc forms the basis for the real-time computing facility developed at the University of California at Santa Barbara under the direction of Professor Duncan A. Mellichamp. High speed paper tape input/output and a medium speed line printer facilitate programming and operations. Sixteen channels of A/D and 8 channels of D/A conversion are available along with 16 lines each of binary data sense and control.

The computer facility has been designed to operate in the department process dynamics and control laboratory. It is permanently interfaced to the department analog computer facility and also can be connected (via replaceable patch panels) to four undergraduate experiments demonstrating unsteady liquid level control and stirred-tank energy transfer. Timesharing software is available to permit undergraduate students to operate all of these experiments simultaneously from the computer.

Additionally, two experiments especially designed to demonstrate the important features of digital computer monitoring and control were built for a new undergraduate elective course in real-time digital computing. One, utilizing pressure control as a demonstration, makes use of binary inputs (solenoid valves) and outputs (pressure relays) to illustrate binary data handling and logic. The second, involving heat transfer in a heated bar, is used to demonstrate multi-point data logging and, also, direct digital control.

Several graduate research processes presently are interfaced to the computer including a multi-input/multi-output heat exchanger and an autothermal catalytic reactor.

CACHE COMMITTEE FUNDED BY NSF FOR CONTINUED SUPPORT

The CACHE Committee has learned recently that its proposal for continued support beginning in the Spring of 1973 has been approved by the National Science Foundation. Funds have been budgeted and will be released to the National Academy of Engineering as needed to complete specific CACHE projects. The NAE received an award from NSF in January, 1971 for an initial two-year period. During the next phase of CACHE Committee activities, the committee will be focusing upon the use of new computing technologies in the preparation and dissemination of computer-based instructional materials.

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. The person to contact for further information about any event is indicated in parenthesis.

April 6, 1973, EDUCOM Spring Conference, Harvard Business School, Cambridge, Mass. In the afternoon from 1:45 p.m. to 3:45 p.m. there will be a workshop on chemistry and chemical engineering resources for networking held as part of the conference at the MIT, Dept. of Chemical Engineering. (For further information, contact Prof. L. B. Evans, Dept. of Chem. Eng., MIT, Cambridge, Mass. 02139, Telephone: (617) 253-4580).

April 24-28, 1973, European Federation of Chemical Engineering will hold an International Congress on the Use of Electronic Computers in Chemical Engineering in Chatenay-Malabry (near Paris) at l'Ecole Centrale des Arts et Manufacturers. (For further information contact: Société de Chimie Industrielle, 80 Route de Saint Cloud. 92—Rueil Malmaison, France.)

June 3-16, 1973, Continuing Education Course on "Digital Computers in Chemical Instrumentation" (Dr. S. P. Perone, Chemistry Dept., Purdue Univ., Lafayette, Ind. 47907)

June 18-19, 1973, Engineering Summer Conference on "Modern Methods for Solving Engineering Problems: Numerical Methods, Optimization Techniques, and Simulation," University of Michigan, Ann Arbor, Michigan 48105. (Professor Brice Carnahan, telephone 313-764-2383)

June 20-29, 1973, 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 617-253-4580)

August 27-31, 1973, Short Course on "Analysis of Chemical Process Design Alternatives Using the Computer," University of Pennsylvania, Philadelphia, Pennsylvania 19174. (Prof. W. D. Seider, telephone 215-594-7953).

September 9-12, 1973, AIChE-C.S.Ch.E. 4th Joint Meeting, Vancouver.

Symposium on Computer-Aided Design in Pollution Control (L.T.Fan, Dept. of Chem. Eng., Kansas State Univ., Manhattan, KA 66502).

Symposium on Process Dynamics and Control and Real-Time Computing (D.G. Fisher, Dept. of Chem. and Pet. Eng., Univ. of Alberta, Edmonton, Alberta).

Symposium on Computer Needs and Applications in the Process Industry (R.S.H. Mah, Dept. of Chem. Eng., Northwestern University, Evanston, III. 60201).

Symposium on Management of Computers (M.T. Tayyabkhan, Mobil Research and Development Corp., P.O. Box 1026, Princeton, N.J. 08540).

Symposium on Shared Teaching Experience (D.R. Woods, Dept. of Chem. Eng., McMaster Univ., Hamilton, Ont.).

November 11-15, 1973, AIChE 66th Annual Meeting, Philadelphia. Symposium on Advances in Chemical Engineering Computing (A.W. Westerberg, Dept. of Chem. Eng., Univ. of Florida, Gainesville, Fla. 32601).

March 10-13, 1974, AIChE 76th National Meeting, Tulsa. Symposium on Optimization Theory and Applications (R.W. Pike, Dept. of Chem. Eng., Louisiana State Univ., Baton Rouge, La. 70803).

Symposium on Computer-Aided Process Synthesis (J.D. Seader, Univ. of Utah, Dept. of Chem. Eng., Salt Lake City, Utah 84112).

Symposium on Reservoir Analysis and Simulation by Computer (M.R. Tek, Dept. of Chem. Eng., Univ. of Mich., Ann Arbor, Mich. 48105).

July 18-19, 1974, 1973 Summer Simulation Conference, Montreal. (Lawrence Sashkin, The Aerospace Corp., P.O. Box 92957, Los Angeles, California 90009)

LOCAL CACHE REPRESENTATIVES DESIGNATED

An attempt has been made to designate one individual at each chemical engineering department in the United States and at many foreign universities as the official representative of their institution for liaison with the CACHE Committee. Over 120 individuals have agreed to serve in this capacity for an initial two-year term to expire at the end of the 1972-73 academic year. They receive copies of all publications of the CACHE Committee and bring them to the attention of interested individuals in their department. They also provide a feedback mechanism to the CACHE committee to inform the committee about work at individual schools, to let the committee know whether its activities are of benefit to the general chemical engineering community, and to propose new projects for the committee to undertake. A current list of the local representatives is published below. Any corrections or additions to this list should be reported to Professor Lawrence B. Evans, Room 12-135, MIT, Cambridge, Mass. 02139.

CACHE REPRESENTATIVES

Representative

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