CACHE NEWS

News About Computers
In Chemical Engineering
Education.

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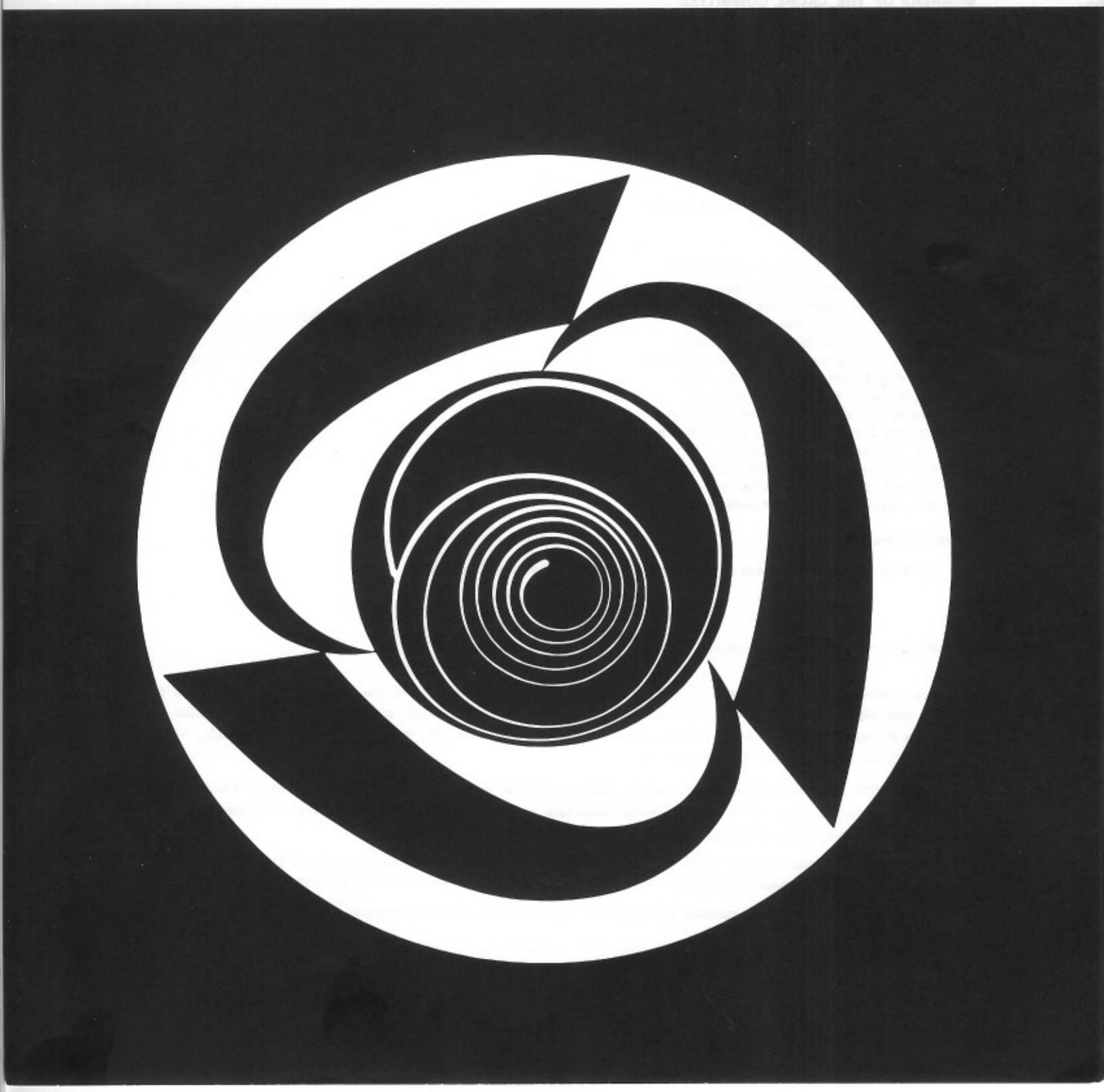

PURPOSE OF THE CACHE COMMITTEE

The CACHE (Computer Aids for Chemical Engineering Education) Committee was established by the National Academy of Engineering' 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 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 12-104, M.I.T., Cambridge, Mass. 02139 (Telephone 617-864-6900 ext 4580 or 4561).

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

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ABOUT THIS NEWSLETTER

This first edition of the *CACHE Newsletter* is being sent to all chemical engineering faculty members in the United States. Anyone who wishes to receive future editions of the *Newsletter* must complete and return the form on the last page.

CACHE COMMITTEE IS ESTABLISHED

A panel of chemical engineering educators called the CACHE (Computer Aids for Chemical Engineering Education) Committee has been established by the National Academy of Engineering's Commission on Education. The purpose of the committee is to coordinate and encourage the development of computing systems for use in chemical engineering education. The National Science Foundation has provided a grant to support the activities of the CACHE Committee for a two-year period.

The 17 members of the committee are drawn from universities throughout the United States and Canada. Each member is actively concerned with the use of computers in chemical engineering and many of them have pioneered in development of computer systems for simulation and design of chemical processes.

The principal goal of the committee will be to accelerate the integration of digital computation into the chemical engineering curriculum by promoting inter-university cooperation in preparation of new courses, teaching aids, and computing systems.

Although there are no representatives of industry on CACHE, the committee plans to have close liaison with industry and to involve people from industry as members of its task forces. Many of the proprietary computer systems developed by industry for process simulation, design, and control have great untapped potential for use in education. Industry also has a special interest in the work of the CACHE Committee, because the ultimate benefit of accelerating use of computers in engineering education is to produce engineering graduates with the training to better meet the needs of industry.

FIRST FORMAL MEETING OF CACHE COMMITTEE HELD IN APRIL

The first formal meeting of the CACHE Committee was held at the University of Michigan in Ann Arbor on April 2-3, 1971. The members of the committee had been meeting informally and working together for the previous two years (see following item). At the meeting in Ann Arbor the committee elected Warren D. Seider chairman, Lawrence B. Evans vice chairman, and Arthur W. Westerberg secretary.

Others present in addition to the 17 committee members included Dr. Newman Hall (an ex-officio member of CACHE) and Mrs. Jean P. Moore of the NAE Commission on Education, Prof. Yi Hua Ma of Worcester Polytechnic Institute, Prof. Edward J. Freeh, Ohio State University, Prof. Ronald L. Klaus, University of Pennsylvania, and Prof. John M. Woods, Purdue University.

Five subcommittees have been established to direct CACHE projects in specific areas related to the use of digital computers in chemical engineering education. The name, mission, and members of each subcommittee are as follows:

1. Standards Subcommittee—to develop mechanisms for standardization of computer programs, system conventions, documentation, and terminology so as to facilitate inter-university interchange of computer programs (P. Shannon, Chairman, E. Grens, R. Hughes, and R. Klaus).
2. Curriculum Subcommittee—to study and develop ideas for effective use of the computer in existing chemical engineering courses and for changes in curricula to exploit new uses of the computer (E. Henley, Chairman. A. Westerberg, M. Reilly, J. Christensen, and R. Jelinek).
3. Physical Properties Subcommittee—to plan and develop methods of integrating computer-based methods for estimation and retrieval of thermodynamic, physical, and transport properties into the undergraduate curriculum, for all courses which would require access to such data (R. Motard, Chairman, W. Seider, and N. Hall)
4. Dynamic Systems Subcommittee—to consider the use of the computer for studying the dynamic behavior of interacting chemical processes, to coordinate work on computer systems under development, to carry out studies of current use, to undertake teaching experiments and to make recommendations for incorporation of these dynamic systems in undergraduate classes in control and design (A. Johnson, Chairman, R. Weaver, I. Zwiebel, E. Freeh, and D. Woods)
5. New Projects Subcommittee—to consider use of computing in the chemical engineering curriculum in areas which are undergoing very active stages of research, such as on-line monitoring and control of chemical process apparatus, computer-aided chemical process synthesis, and computer graphics (L. Evans, Chairman, B. Carnahan, E. Elzy, and J. Seader).

The activities planned by each subcommittee will be described elsewhere in the *Newsletter.*

Dr. Newman Hall remarked at the Ann Arbor meeting that "The most important challenge facing CACHE will be to find ways to achieve an impact on the chemical engineering programs at a large number of universities in addition to those represented by CACHE Committee members." The committee has already invited several additional people to serve on various subcommittees and task forces and many more will be involved as on-going projects develop.

ORIGINS OF CACHE COMMITTEE BEGAN IN 1969

The idea to establish a committee such as CACHE originated with Professors Carnahan, Motard, and Seider who organized the first meeting of interested chemical engineering faculty members in Ann Arbor in April 1969. They wished to create a committee patterned after the COSINE (Computers in Electrical Engineering) Committee which is also sponsored by the NAE Commission on Education and which

conventions, data formats, and documentation have been responsible for duplication of effort at different schools. CACHE has established a Standards Subcommittee to devise mechanisms for facilitating easier inter-university interchange of computer programs.

The subcommittee has people looking at the problem of setting standards for programming, documentation, program testing, and large-scale systems (such as PACER, CHESS, APPES, etc.). They are also attempting to compile a glossary of computer-related terms which are unique to chemical engineering.

In the course of its work, the CACHE Committee expects to obtain a considerable number of computer programs and systems which have potential use in education. The Standards Subcommittee is attempting to develop an effective policy and mechanism for distributing the programs.

An important question facing the subcommittee is, how should standards be implemented? Some of the problems in introducing standards are that it is difficult to get agreement on a standardization procedure, they may discourage people from contributing programs because of the effort to bring them up to the standards, and they could conceivably stifle creativity in developing nonstandard ideas. On the other hand without standards it is virtually impossible to transfer computer programs from one computer to another and there is considerable wasted and duplicated effort.

Professor Paul Shannon, chairman of the Standards Subcommittee, is well aware of the problems and commented that "the task of setting standards is formidable!". He would appreciate a letter or telephone call (at 603-643-4440) from anyone who has suggestions or wishes to work with the subcommittee.

CACHE TO SURVEY REAL-TIME COMPUTING

The digital computer is seeing increased use for on-line monitoring and control of chemical process apparatus. The computer can be used to monitor experiments in the unit operation laboratory as well as in graduate research programs. Another important application is in the process control laboratory where the on-line computer is used for direct-digital feedback and feedforward regulation, for supervisory control, and for automatic start-up and shut-down.

There is essentially no coordination of the effort in this field that is going on at different universities. The extent of existing and proposed programs is unknown. There appear to be few guidelines to selection of appropriate hardware and software and to the integration of real-time computing into the curriculum.

To gather some much-needed information, the New Projects Subcommittee is surveying the nature and extent of the use of real-time computing at colleges and universities in the United States, Canada, and Great Britain. A letter was sent to all chemical engineering department heads in these countries on May 3, 1971 and within the first month responses were received from about 50% of those contacted. Results of the survey will be published in a future issue of the *Newsletter* and will be used to guide the subcommittee's activities in this field.

It is tentatively planned to hold a workshop on real-time computing in the chemical engineering laboratory sometime during the academic year 1971-72. An invitation would be extended to every chemical engineering department which is either currently using the real-time computer or plans to begin using real-time computing to send one or more representatives to the workshop.

The workshop would cover a variety of aspects of the use of the real-time computer, including advantages and disadvantages of various hardware and software configurations, types of experiments to be connected to the computer, method of introducing its use into the curriculum, etc.

Anyone who wishes to become actively involved in the CACHE Committee activities in the field of real-time computing should contact Prof. L. B. Evans, Chairman of the New Projects Subcommittee.

SYMPOSIUM AT DALLAS TO FEATURE COMPUTER-AIDED PROCESS SYNTHESIS

A symposium on Computer-Aided Process Synthesis has been recently added to the program for the 71st National Meeting of the A.I.Ch.E. to be held in Dallas, Texas, February 20-23, 1972. The CACHE Committee took the initiative in organizing this symposium; Professor J. D. Seader of the University of Utah and Professor E. Elzy of Oregon State are co-chairmen. Anyone who wishes to participate in the symposium should contact Professor Seader.

Although the computer has been used for process simulation for a long time, the development of techniques for computer-aided process synthesis is a relatively new phenomenon. A survey conducted in 1970 by Professor Seader for the CACHE Committee revealed that interest in the process synthesis aspect of process design is growing and that innovative work was underway at several institutions.

Unfortunately, about 25% of the persons responding to the survey were uncertain as to what was meant by the term *process synthesis.* Professor Seader admits "This term has not had widespread usage or adoption and perhaps there is no consensus concerning a strict definition." He defines process synthesis as "the creation of a processing scheme for converting raw materials to more valuable or desirable products."

A process synthesis may be displayed in the form of a process flow diagram which shows all major items of equipment including reactors, component separation devices, heat exchangers, compressors, pumps, phase separators, etc. The synthesis may also include the preliminary determination of nominal operating ranges of temperature and pressure at key steps in the process. In general, process synthesis, according to Professor Seader's definition, must precede the application of computer-aided process simulation or design programs such as CHESS, PACER, AND FLOWTRAN. The user of these computer programs must supply the synthesis or processing scheme.

The New Projects Subcommittee of CACHE is actively concerned with methods of introducing new developments in computer-aided process synthesis into the chemical engineering curriculum. Anyone who is interested is invited to join in the work of the subcommittee and is encouraged to contact Professor Seader.

SUBCOMMITTEE TO SURVEY PROPERTIES

An important feature of chemical engineering is its need for data on the properties of a wide variety of pure materials and mixtures. CACHE has established a subcommittee chaired by Professor R. L. Motard of the University of Houston whose primary objective is the integration of computer-based estimation and retrieval methods for thermodynamic, physical, and transport properties into the undergraduate curriculum.

The subcommittee feels that there is an important need for a critical bibliography of data, existing programs and estimation methods. A number of large computer-based systems have been developed at universities and in industry for physical property estimation and retrieval. A major problem with such systems, however, is keeping them flexible, easy to use, extensible, and transportable from one organization to another.

The first item on the agenda for the subcommittee will be to ascertain the needs for physical property programs in chemical engineering education and to evaluate concepts and available software for developing physical property data systems suitable for university use. The subcommittee plans to convene a meeting this summer of noted experts and interested educators to refine its objectives and formulate a plan of action. Anyone who is interested in this area and willing to work with the subcommittee is encouraged to contact Prof. Motard.

CALENDAR OF EVENTS

The Calendar of Events will be a regular feature of the *Newsletter*; it will list 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.

June 20-24, 1971 Annual Meeting of ASEE, Annapolis, Maryland

A half-day session on the use of the computer in chemical engineering education is scheduled for June 22. (W. D. Seider, School of Chem. Eng., 376 Towne Building, University of Pennsylvania, Philadelphia, Pa. 15213.)

June 21-July 2, 1971

Special Summer Program on "Numerical Methods optimization Techniques, and Simulation for Engineers" University of Michigan, Ann Arbor Tuition: $425 with scholarships for faculty members (Prof. B. Carnahan, tel. 313-764-4466).

June 22-July 1, 1971

Special Summer Program on "New Developments in Modeling, Simulation, and Optimization of Chemical Processes," Massachusetts Institute of Technology, Cambridge, Mass. 02139 Tuition: $450 with scholarships for faculty members (Prof. L. B. Evans, tel. 617-864-6900 x4580 or 4561).

July 19-23, 1971

1971 Summer Computer Simulation Conference, Boston, Mass. Sponsored by the ACM, AIAA, AIChE, AMS, BSC, IEEE, ISA, Sci, SHARE. (General Chairman: Takeshi Utsumi, Stone and Webster Eng. Corp, P. O. Box 2325, Boston, Mass. 02107).

August 29-September 1, 1971 A.I.Ch.E. 70th National Meeting, Atlantic City

Symposium on Chemical Engineering Computing: Overview—the Future (E. H. Blum, New York City Rand Institute, 545 Madison).

November 28-December 2, 1971 A.I.Ch.E. 64th Annual Meeting, San Francisco

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

*Seminar on Dynamic Systems and Control in the Undergraduate Chemical Engineering Program. (A. I. Johnson, Dept. of Chemical Engineering, McMaster University, Hamilton, Ontario, Canada).

February 20-23, 1972 A.I.Ch.E. 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, Dept. of Chem. Eng., Louisiana State Univ., Baton Rouge, La. 70803).

Symposium on Use of computers in the Educational Process (J. J. Lagowski, Dept. of Chemistry, Univ. of Texas, Austin, Tex. 78712).

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

May 21-24, 1972 A.I.Ch.E. 72nd National Meeting, St. Louis

* Symposium on CACHE Update—Computer-Aided Chemical Engineering Education (W. D. Seider, School of Chem. Eng., 376 Towne Building, Univ. of Pennsylvania, Philadelphia, Pa. 15213).

Symposium on Plant Applications of Computers (C. W. DiBella, Monsanto Co. 800 N. Lindbergh Blvd., St. Louis, Mo. 63166).

Symposium on Advances in Process Optimization (V.J. Law, Dept. of Chem. Eng., Tulane Univ., New Orleans, La. 70118).

Auguest 27-30, 1972 A.I.Ch.E. 73rd National Meeting, Minneapolis

Symposium on Applied Numerical Methods (M. R. Samuels, Dept.of Chem. Eng., Univ. of Delaware, Newark, Del. 19711).

November 26-30, 1972 A.I.Ch.E. 65th Annual Meeting, New York City

Symposium on Advances in Chemical Engineering Computing (M.T. Tayyabkhan, Mobil Research and Development Co., P.O. Box 1026, Princeton, N. J. 08540).

March 11-15, 1972 A.I.Ch.E. 74th National Meeting, New Orleans

Symposium on Optimization Theory and Applications (R. W. Pike, Dept. of Chem. Eng.m Louisiana State Univ., Baton Rouge, La. 70803).

. . . TO RECEIVE FUTURE ISSUES OF THE *NEWSLETTER*

Anyone who wishes to receive future editions of the *CACHE Newsletter* must complete and return the form below:

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