

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

TECHNICAL COMPUTATIONAL NEWSLETTER

Sigmund J. Lawrence, Editor

First Quarter, 1976

EXCERPTS FROM THE ANNUAL REPORT, FEB. 16, 1976

This newsletter is a new endeavour of the Machine Computation Committee. The purpose is to disseminate technical news about computing and its chemical engineering applications; to tell what is happening - meetings, conferences, new books, including announcements of future events and review of past events; to inform readers of MCC news and member activities.

Each issue will contain at least one major technical news item, reflecting the experience of the writer. There will be three or four issues per year with no firm publishing deadlines. We will recognize our responsibility to authors to publish their material promptly.

For the first year, this newsletter will be sent to MCC members, those responding to the MCC 1975 questionnaire and AIChE's Code 77 (computer-interested) members.

Articles should be submitted to the editor. (See editorial for address).

EDITORIAL

We begin humbly, cautiously, with this first newsletter of the Machine Computation Committee. We hope to fill a need with its dissemination. We will be guided by the reactions of you, the reader. Therefore, send your comments to the editor, at 10 Yorkshire Drive, East Windsor, NJ 08520.

With the birth of this newsletter, I must share the joy of another birth with you: Mary Aleksandra, born January 17, at 7 pounds, 9 ounces.

If you feel the urge to call me, my office phone is 215-864-3861, and my home phone is 609-443-5827.

Sig Lawrence

Present Machine Computation Committee (MCC) membership is 57, as compared with 34 at the end of last year. This increase is due partly to the advertising for help in CEP and partly to the increased visibility arising from the increased activity. The Committee met in Houston (March), Boston (September), and Los Angeles (November). The last two meetings included lunch with attendance of 9, 14 and 23, respectively.

In 1975, there was some real growth in MCC, although we have not yet reached the plateau of constructive activity that we have had our sights set on for the last year. The organizational structure continues as before: members contribute to the activities in which they have a special interest or valuable experience and the leadership comes from the most interested member of the group, all on an ad hoc basis. MCC officers for 1976 are:

Charles H. Ware, Jr., Chairman;
Vernon J. Sterba, Vice-Chairman; and Warren D. Seider, Secretary-Treasurer. A third officer was added to aid in the continuity of leadership and the treasurer's duties were added to handle the budget that was established for MCC. In 1976, the MCC meetings will be held at the Kansas City, Atlantic City, and Chicago meetings.

Vern Sterba will continue as Membership Chairman in addition to MCC Vice-Chairman. Warren Seider will continue as our representative to the Program Committee, Area 1d, in addition to MCC Secretary-Treasurer. Ted Peterson is the Chairman of Group 1. A total of 11 technical sessions were held, 4 in computing and the rest in applied math. In 1976, 8 sessions in computing and 1 in applied math are planned.

Dick Hughes is editor of the new journal, "Computers and Chemical Engineering". Ron Klaus is Special Feature Editor, and is in charge of the review of computer programs and their descriptions which will appear in the journal. A firm publication date has not been set. This publication project will supercede the Swap Shop.



Alan Glueck is preparing the MCC portion of the AIChE Journal review. Ted Leininger is coordinating liaison with computer groups outside of AIChE. Because of the lack of MCC member interest in the Summer Simulation Conferences, the committee has recommended, and Council has approved, to end MCC participation.

National Center For Chemical Engineering Computing

MCC has begun formal consideration of such a center. Two panel discussions were organized by Charlie Ware with Warren Seider, and an ad hoc committee has been organized under the direction of Rudy Motard. Two "Institute News" articles have been written for CEP (October '75 and March '76). Close liaison exists between MCC and national computing center groups in ACS and ASCE. A decision is expected at the Kansas City meeting regarding the direction we would like to explore and how we will do so.

Division Status

Bob Morris heads up a committee comprised of former MCC Chairmen to prepare a proposal for the formation of a division.

The 1975 Annual Report of the Machine Computation Committee has been mailed to committee members. Non-members may obtain a free copy by writing to the chairman:

Dr. Charles H. Ware, Jr., Commercialization Insights, 33 Sandi Drive, Poughkeepsie, NY 12603

INFORMATION GOODIES FROM THE EJC

The Engineers Joint Council will complement its existing Guide to Engineering Information Sources with a directory listing the many numerical and graphical data basis or centers available for commercial use. Prior to this time, there has been no central directory listing them.

The EJC Commission on Engineering Information has undertaken this new project, as announced by Edward A. Ledeen, Manager of Information Programs for EJC, at the Nov. 1975 Conference on Energy Information Tools sponsored by the Information Industry Association and the National Federation of Abstracting and Indexing Services. For information on the new directory, contact Edward Ledeen at (212) 644-7842.

The Guide to Engineering Information Sources provides "where to find it" information on all major fields of engineering plus closely allied subjects. It is a pocket-sized folder which will enable the engineer, technician, scientist, economist, etc. to find an organization having specific knowledge of the area in question. Details on the Guide can be had by calling (212) 644-7840.

If you wish to order Guides, send your order to: Commission on Engineering Information, Engineers Joint Council, 345 East 47th Street, New York, NY 10019, with your check. There is a \$1.00 charge for billing. Bulk shipments can be ordered in accordance with the price schedule below.

1-499	50¢ each
500-999	40¢ each
1000-and up	25¢ each
Minimum Order	\$10.00

SOFTWARE PACKAGES EVALUATED

The December 1975 issue of Datamation features an article entitled, "User Ratings of Software Packages". In it, 211 software packages are rated and 25 of them are listed the "1975 Software Honor Roll". Detailed results of the survey described in the article are contained in "User Ratings of Proprietary Software", a 36 page DATAPRO 70 report available for \$10.00 from Datapro, 1805 Underwood Boulevard, Delran, NJ 08075 (609) 764-0100.

MCC QUESTIONNAIRE FOR 1975

A Machine Computation Committee questionnaire was conducted in 1975 by Vernon J. Sterba and James Eakman. There were several objectives:

- 1) To find likely candidates for reviewing papers.
- 2) To find likely candidates to present papers on the interdisciplinary areas which involve chemical engineers.
- 3) To make relevant programs at national meetings more effective.
- 4) To alert interested engineers about such coming programs.

Among other things, the questionnaire was arranged to provide five choices of professional interest from a listing of thirty-two classifications.

Warren D. Seider'

Each classification was divided into nine subclasses. Seventy responses were obtained from a mailing to approximately 330 engineers, including the MCC, which numbers 57. Results for the total in each major classification is shown below.

Chemistry	17
Physics	0
Thermodynamics	11
Gas Absorption/Stripping	0
Distillation	21
Extraction	1
Solids Contacting	1
Specialized Separations	0
Fundamental Fluid Mechanics	6
Applied Fluid Mechanics	3
Heat Transfer Fundamentals	1
Applied Heat Transfer	13
Solids Handling	0
Size Reduction and Enlargement	1
Kinetics	10
Chemical Reactor Analysis	10
Process Engineering	30
Project Engineering	14
Plant Engineering	0
Instrumentation	8
Control Theory and Practice	25
Process Dynamics	36
Applied Mathematics	29
Computation	65
Materials-Metallurgy	1
Materials-Organic	5
Materials-Inorganic	0
Materials-Biological	2
Bioengineering	1
Environmental Engineering	3
Economics/Finance	25
Management/Business	11

The idea of selecting more than one field of interest is not new. However, thru this experience, perhaps additional direction may be provided for revision of AIChE questionnaires which permit only one choice.

A second mailing is planned which will include the one thousand AIChE "Code 77" members -- those whose chemical engineering specialty is computation.

Have a Happy $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$

Have you considered the use of large software systems and data bases developed by others? If so, you are probably familiar with rapidly expanding computer networks. The objective of this article is to discuss the role of computer networks in software distribution.

Most of us are familiar with one or more aspects of the following scenario. The XYZ computer system, Version 1, has been released and is available for installation on in-house computers. It is comprised of 30,000 FORTRAN statements, 100 subroutines, and numerous data records organized in a data base. Chemical Engineer A would like to use the system, but is reluctant to undertake the time-consuming and routine task of system maintenance. He contacts Chemical Engineer B, a computer specialist, to suggest the possibility of the computer department maintaining the system. If the right combination of circumstances exists - that is, (1) a "critical mass" of users can be found, (2) a home-grown system does not exist, and (3) the computer department has the expertise to maintain the system - the system will be installed and maintained.

More often as software systems become more specialized, a critical mass of users cannot be found within a single company. Two examples are (1) engineers in an inorganic chemical company which is diversifying into petrochemicals, with different equipment requirements, and (2) engineers in any company which does little of its own design work and, therefore, does not have a computer-aided design capability. Yet, these chemical engineers need to access these packages as simply and reliably as they access mini-computers and pocket calculators.

The heirarchical computer network is designed to reach widely distributed users and offers the facilities to resolve the critical mass problem. Such a network consists of at least one large-scale computer (e.g., IBM 370/168, CDC 7600, and UNIVAC 1110) linked to a communication network (e.g., Bell Telephone System with mini-computers to package large quantities of data for transmission over leased lines). The communication network permits typewriter terminals,

card reader - line printer terminals, and local computers to communicate with the large-scale computer. Specialized software and data bases are installed on the large-scale computer and maintained by a staff of experts. The geographical distribution of access points to the communication network must be sufficiently broad to create a large enough user community to reduce the communication costs per user.

An important requirement is that users be able to insert their personal subroutines and data records into a private library on the large-scale computer. Local computers would be used to prepare and test the subroutines and data prior to insertion on the large-scale computer. It should also be possible to retrieve selected subroutines and data from the large-scale system for use on a local computer. This feature is not usually available today, since most large-scale systems are not easily decomposed into modules that can be used independently of each other. Next generation systems are being designed to be more modular and more easily decomposed.

In the spring of 1974, the CACHE (Computer Aids for Chemical Engineering Education) Corporation's Program Distribution Task Force undertook a study of computer networks when Monsanto Co. generously agreed to make FLOWTRAN available for training at universities. The Task Force examined several networks including ARPANET, CYBERNET, General Electric, INFONET, and United Computing Systems (UCS). To assist in evaluating the networks, the Task Force prepared a document entitled "CACHE Guidelines for Computer Networks" (available from CACHE, Room 12-188, 77 Massachusetts Ave., Cambridge, Mass. 02139). It lists ten guidelines for the host computer regarding input, output, accounting, technical support, literature, cost, and reliability. The five guidelines for the communication network itself cover communication speed, costs, accessibility and simplicity in use.

CACHE selected the UCS Network. Other networks offer similar arrangements for communication with typewriter terminals (300 baud lines = 30 characters per sec.), but UCS was judged to be accessible to more

schools for the cost of a local phone call. In addition, UCS provides an 800 exchange (toll-free lines) for 2000 baud communications from anywhere in the United States. The first year of experience has shown that most chemical engineering departments are communicating with UCS over these lines using medium speed terminals with card readers and line printers.

Several sequences of control cards have been established to access the FLOWTRAN programs and data base on the UCS CDC 6600 computer. Prof. Richard R. Hughes (Univ. of Wisconsin) found it helpful to prepare a manual to describe the techniques for using UCS facilities in accessing FLOWTRAN. The manual, entitled "CACHE Use of FLOWTRAN on UCS", is available from the CACHE office at a cost of \$1.00.

For persons interested in learning more about computer networks, the following references are recommended:

1. Blanc, R.P., Review of Computer Networking Technology, NBS Technical Note 804, National Bureau of Standards, 1974.
2. Cornew, R. W. and P. M. Morse, "Distributive Computer Networking: Making it Work on a Regional Basis," Science, 189, August, 1975.
3. Doll, D.R., "Computer Networking - The Giant Step in Data Communications", Data Communication Systems, Sept., 1973.

