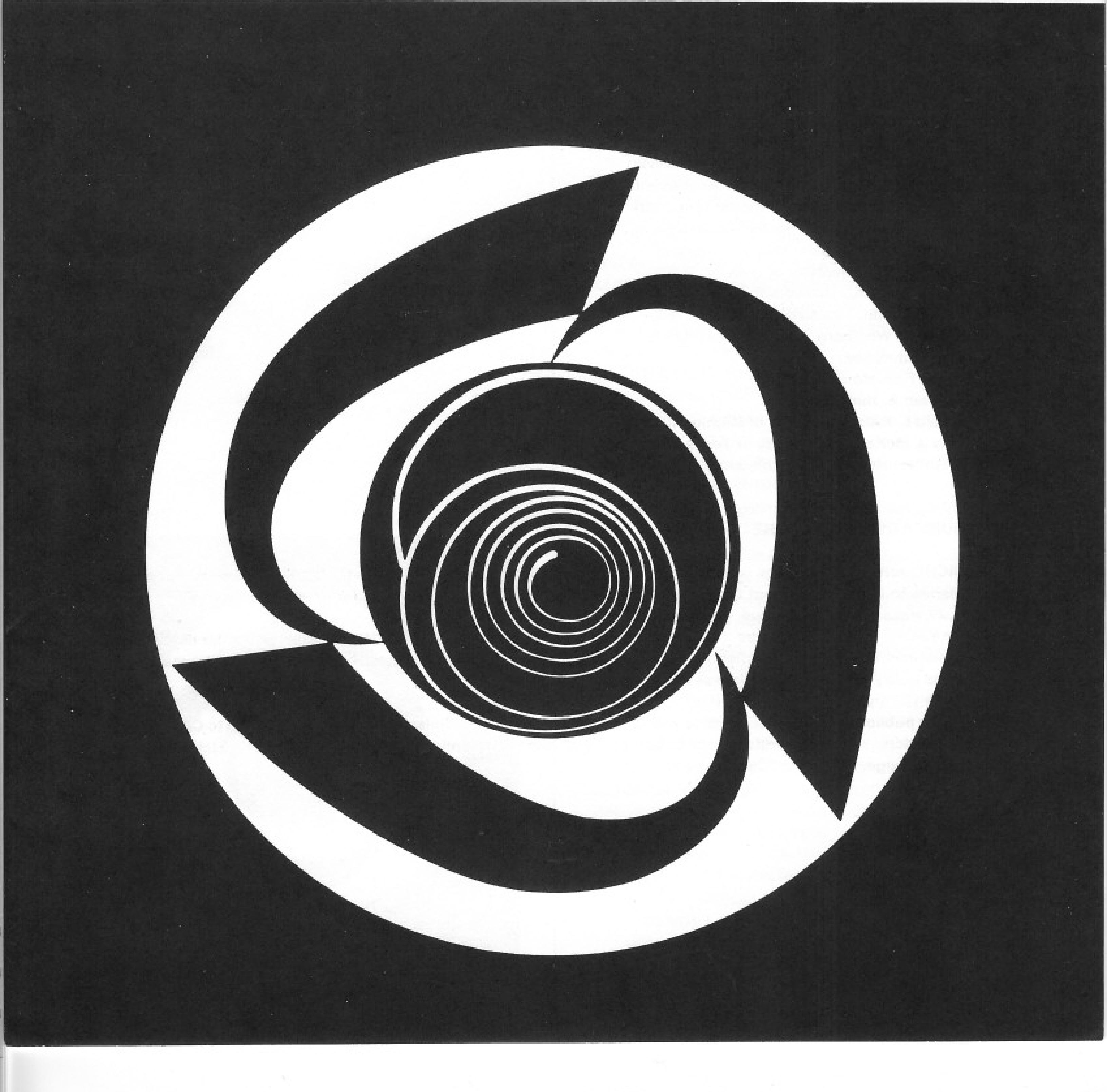
CACHE NEWS

No. 5

News About Computers In Chemical Engineering Education.

May, 1976



PURPOSE OF CACHE

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

MEMBERS OF CACHE

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 ELECTS NEW OFFICERS

At the CACHE Semiannual Meeting held outside Kansas City in April, Robert Weaver (from Tulane University, now visiting professor at MIT) was elected CACHE's new President. CACHE's new Vice-President is Prof. Duncan Mellichamp of the University of California, Santa Barbara; and Prof. Rodolphe Motard of the University of Houston has been elected incoming Secretary. CACHE's headquarters in Cambridge will continue to be directed by our Executive Officer, Prof. L. B. Evans of MIT. The officers welcome contacts from CACHE departmental representatives, from Department Chairmen, and from industrial associates for information and for comment on current and potential CACHE initiatives.

CACHE CONTINUES TO RECRUIT BROADER INVOLVEMENT IN TASK FORCE ACTIVITIES

CACHE has continued to find the infusion of new talent into the Board of Trustees and into its Task Force Activities a source of valuable new ideas and perspective. Normally, new Trustees have been drawn from active participants in the various projects and it is with an eye to future as well as to meet present objectives that CACHE actively seeks new participants in its project activities. Departmental representatives and Department Chairmen can assist us a great deal in locating this talent and this input is earnestly solicited. Suggestions can be directed either to the Vice-President (Professor Duncan Mellichamp, University of California, Santa Barbara) or to the respective task force chairman listed below:

- ChE Modular Instruction Project (CHEMI): Prof. Ernest Henley (University of Houston)
- Program Distribution and Large Scale Systems Projects (FLOWTRAN, et al.):
  Prof. Warren Seider (University of Pennsylvania) and
  Prof. J. D. Seader (University of Utah)
- Real Time Computing Project: Prof. Joseph Wright (University of Alberta, Edmonton)
- Physical Properties Projects: Prof. Rodolphe Motard (University of Houston)
- Resource Management Project: Prof. Robert Weaver (Tulane University, currently at M.I.T.)
- Computer-Aided Graphics: Prof. Richard Mah (Northwestern University, Evanston)

ANNOUNCEMENT OF FORTHCOMING ELECTION OF CACHE TRUSTEES

The election of new Trustees to the CACHE Corporation will be held at the Corporation's Annual Meeting in November. Nominations should be presented to the Vice-President by October 1, 1976. This nominating letter and a brief accompanying biographical resume should be addressed to:

Professor Duncan A. Mellichamp
Department of Chemical and Nuclear Engineering
University of California
Santa Barbara, California 93106

THE CHEMI PROJECT

In the November 1975 *CACHE Newsletter*, the CHEMI (Chemical Engineering Modular Instruction) Project was described. Briefly recapping the article, the NSF funded project (begun in July 1975) is commissioning the preparation of small, self-study, fundamental concept modules for the various areas of undergraduate chemical engineering. From fifty to one hundred modules are envisioned in each of seven curriculum areas: Control, Transport, Stagewise Processes, Design, Material and Energy Balance, Kinetics, and Thermodynamics. Also, a means of distribution of these modules to the entire chemical engineering community is being established.

To date, the response to the project has been enthusiastic and encouraging. About 80% of the modules have been commissioned. While most of these have first draft deadlines of Aug., 1976, some have already been completed. The remaining 20% are available for authorship. A listing of these interesting modules is included at the end of this article. We would like to invite you to join us in this new venture in education by authoring one or more of these available modules. The following recognition and compensation will be given to module authors:

1. Wide distribution of your module to the chemical engineering community with identification of author and institution in the copy and on the cover.
2. Announcement of the availability of your module in the *CACHE Newsletter* and in periodic news releases to chemical engineering journals.
3. $50.00 honorarium for each module.
4. The review process is designed to enhance the professional recognition of your work and to make it comparable to that of research articles.

If you would like to write any of these modules, or suggest others, please write directly to the Editor-in-Charge. Addresses are given below.

Kinetics Billy Crynes, Ch.E. Dept., Oklahoma State University, Stillwater, Oklahoma 74074 or Scott Fogler, Ch.E. Dept., University of Michigan, Ann Arbor, Michigan 48104

Thermodynamics Bernie Goodwin, Ch.E. Dept., Northeastern University, Boston, Massachusetts 02115

Control Tom Edgar, Ch.E. Dept., University of Texas, Austin, Texas 78712

Stagewise Processes Ernest Henley, Ch.E. Dept., Cullen College of Engineering, University of Houston, Houston, Texas 77004

Transport Ron Gordon, Ch.E. Dept., University of Florida, Gainesville, Florida 32601

Design Robert Jelinek, Dean, School of Environmental and Resource Engineering, State University of New York, Syracuse, New York 13210
or Robert Weaver, Ch.E. Dept., Tulane University, New Orleans, Louisiana 70118

Material and Energy Balances David Himmelblau, Ch.E. Dept., University of Texas at Austin, Austin, Texas 78712

The Project Director is Ernest Henley (University of Houston) and the Assistant Director is William Heenan (University of Puerto Rico). The Steering Committee consists of:

Lawrence Evans Massachusetts Institute of Technology	David Himmelblau University of Texas
Gary Powers Carnegie-Mellon University	Duncan Mellichamp University of California
Ernest Henley University of Houston	Robert Weaver Tulane University

Listing of Available Modules:

STAGEWISE AND MASS TRANSFER OPERATIONS—E. J. HENLEY

1. Degrees of freedom by the description rule
2. Degrees of freedom by design variable method
10. Batch distillation
11. Description of equipment for stagewise contractors
14. Ponchon methods (simple)
16. Distillation column design (mechanical)
16a. Distillation column design—tray efficiencies
17. Packed column design (mechanical)
22. Multicomponent separations—relaxation methods
26. Molecular diffusion in gases
27b. Use of Ks, HTUs and NTUs in design of gas absorbers
35. Choice of solvent in extraction
45. Adsorption

KINETICS—B. CRYNES AND S. FOGLER

B3-2 Temperature sensitivity of rate constants—II
B7-4 Evaluation of rate data—IV
AII-2 Catalyst deactivation—II
AII-3 Catalyst deactivation—III
A13 Classification of catalyst—III
A22 Polymerization kinetics (1 or 2 modules)

PROCESS CONTROL—T. EDGAR

37. Dynamics and control of heat exchangers

THERMODYNAMICS—B. GOODWIN

8. Standard heat of reaction
13. Relations among thermodynamic properties
16. Property calculations involving phase changes including the Clausius-Clapeyron equations
21. Properties of real gas mixtures
33. Internal combustion and jet engines
35. Mechanical Energy Balance
37. Historical background and foundation
41. Irreversible thermodynamics

TRANSPORT—R. GORDON

Momentum Transport

6. Macroscopic momentum and mechanical energy balance

Heat Transport

27. Steady state heat conduction problems in 2 and 3 dimensions
31. Discussion of viscous dissipation term in energy

equations

33. Heat transfer in laminar boundary layers, approximate solution techniques
35. Natural convection
36. Condensation and boiling

Mass Transport

39. Multicomponent diffusion

MATERIAL AND ENERGY BALANCES—D. HIMMELBLAU

1. Units and dimensions (including systems, conversion factors)
2. Methods of analysis and measurement (density, concentration, mole and weight fraction, specific gravity, etc.)
3. General guidelines for solving problems (including selection of basis)
4. Temperature (measurement, scales, conversion)
5. Pressure (measurement, scales, conversion)
6. Sources of data for physical properties
7. Ideal gas laws for one component
11. Real gas computations—mixtures
12. Vapor pressure
13. Saturation, humidity
14. Partial saturation, humidity
15. Phase phenomena (including phase rule)
16. Steady state material balances—algebra not required
17. Steady state material balances—algebraic solutions required (includes the components)
18. Steady state material balances—recycle, bypass, purge
19. Steady state material balances—involving vaporization and condensation
20. Degrees of freedom in process specification
21. Steady state material balances—multiple process of equipment
24. Solution of steady state material balances via the computer—Part III
25. Concepts of energy and work (including heat, kinetic energy, potential energy, state, enthalpy, property)
26. Heat capacity (definition, measurement, computation, prediction)
27. Enthalpy (computation, application, tables, charts)
28. Enthalpy for phase change
29. Steady state energy balance—principle and formulation
30. Steady state energy balance—application
31. Mechanical energy balance
32. Heat of formation, reaction, and combustion
33. Change of heat of reaction with temperature and pressure
34. Incomplete reactions
35. Heats of solution and mixing
36. Steady state simultaneous material and energy balances—principles
37. Steady state simultaneous material and energy balances— applications to combustion
38. Steady state simultaneous material and energy balances—application enthalpy concentration charts
39. Steady state simultaneous material and energy balances—application humidity charts and their use
40. Steady state simultaneous material and energy balances—application to . . .
41. Unsteady state balances—principles
42. Unsteady state balances—solution techniques for ordinary differential equations
43. Unsteady state balances—applications and examples

DESIGN—R. JELINEK AND R. WEAVER

GENERAL CONSIDERATIONS

Types of Designs

3. System vs. component design

INDUSTRY AND MARKET PROFILE

Major Commodities

9. Feedstocks and sources (present vs. future)
10. Products, intermediate, byproducts
11. Relation to regional, national economy

Intermediate and End User Profiles

12. Market Analysis

COST ESTIMATION CALCULATIONS

Data Sources, Reliability, Updating

20. Inflation and relevant indices

PROCESS EQUIPMENT DESIGN

Cost Related Procedures and Examples—Units and Small Plant Cases

29. Phase separation units (4 modules)
30. Heat exchangers (4 modules)
31. Materials storage and movement (4 modules)
32. Control methods and instruments (4 modules)
33. Construction materials selection and fabrication (4 modules)
34. Waste disposal, noise and pollution control (3 modules)

PROCESS OPERATIONS ANALYSIS

Computer-Aided Design

37. Mass and energy computations—basic and advanced
40. Basic concepts and classical method
41. Continuous vs. cyclic operation

Government and Regulatory Profile

49. Labor legislation and "equal opportunity" legislation
50. Forms of business organization and taxation policy
51. Basic provisions of contract law
52. Tort action and liability

Reports and Communications

57. Legal requirements and documents

NEW PROJECT IN RESOURCE MANAGEMENT

A new CACHE initiative in Resource Management dealing with the economic demands being made in the food, energy and minerals areas is under way with particular attention to today's fiscal and environmental settings. Task Force members are being recruited from both inside and outside chemical engineering.

The project aims to provide chemical engineering curricula (and others) with teaching materials which assist in integrating macro-economic considerations in design problems as well as in developing a student body which is knowledgeable and conversant in the obvious public issues involved.

Project objectives include the assembly of modular operations research capabilities (forecasting, allocation, regression, etc.) along with the technical, economic and demographic data base essential in making exercises in these fields credible.

Chemical engineering has an important input to make in this subject area and timely curriculum involvement in it can be viewed as enlightened self-interest. There are still no really good communications vehicles in the field and it is all too easy to miss important centers of activity and interest around the continent. Please urge those who would want to follow the work of the Task Force (at any level of involvement) to drop a line to the CACHE Resource Management Task Force Chairman: Prof. Robert Weaver, MIT 66-469, 77 Massachusetts Avenue, Cambridge, MA 02139.

REAL-TIME TASK FORCE USERS SURVEY

The third survey of Real-Time Users continues to show a rapid expansion of facilities and programs in the real-time area as compared to previous surveys made in 1971 and 1973. The Fall 1975 survey was compiled by Dr. John T. Heibel (Ohio State University) with planning assistance from the task force chairman, Dr. Duncan A. Mellichamp (University of California, Santa Barbara).

The latest survey consisted of 19 multiple response questions which dealt principally with four areas: Status of Departmental Real-Time Facilities, Systems Usage and Personnel, Systems Software, and the Existence of Real-Time Instruction within Departments. New areas covered by the survey included the extent to which microprocessors have been used in chemical engineering education and the availability of support personnel.

A summary of responses is given below. Anyone desiring a copy of the complete survey results may write

Dr. John T. Heibel
Department of Chemical Engineering
Ohio State University
Columbus, OH 43220

Of the departments solicited and responding to the survey, 46 now have real-time computing facilities and 24 do not. Nine respondents state that they will be installing new facilities or expanding old ones in 1976.

One interesting point concerns the number of departments with more than one processor. Within 48 responding departments there are 71 total processors. Nine facilities are of true multi-processor design; the two largest facilities are in chemistry departments which responded to the surveys, one facility with 14 processors and one with 9.

As to preference of manufacturer, Data General and Digital Equipment have each supplied equipment for about one-third of the facilities. The remaining third is split amongst Varian, IBM, and other suppliers.

Concerning the configuration of facilities, most users cited a machine memory size of 16K (the mode), with from 5 to 32 ADC channels, 0 to 4 DAC channels, 16 bits or less of digital input, 32 bits or less of digital output. Six users have industry compatible magnetic tape and 22 indicated that a disk unit for bulk storage was available. Card readers are available on 10 facilities. Thus it appears that the earlier recommendations of the Real-Time Task Force concerning the configuration of a "desirable" real-time facility (one with the flexibility and ease of use afforded by such peripherals as a card reader and with bulk storage based operating systems) are being widely followed. This point is further emphasized when comparing the cost of total facilities: relatively few respondents (3) have a facility worth less than $10,000. Neglecting several extremely large systems, (estimated value on the order of one-quarter to one-half million dollars), the average estimated value was $41,000 per system.

More respondents still utilize their facilities for research (61%) than use them directly or indirectly in teaching activities (42%). Also, most responses indicated that 2 to 3 faculty members in the department use the facilities. In some cases no one uses the system; in only a few cases, over six. The typical number of graduate students using real-time facilities was 3 to 6; the maximum number noted was 40.

One area of technology development which is sure to affect the chemical engineering field is that of microprocessor applications. Eight institutions indicated that they presently are using microprocessors in real-time research. Only three furnish instruction concerning microprocessors.

Since real-time systems clearly are becoming large operations—in some cases more like a small to medium size computer center— the task force was interested in the level of support available within departments. Only 13 of 48 responses noted the availability of a trained technician. Six departments have professional (non-student) programmers.

A question concerning the use of operating systems revealed a very mixed picture: single user paper tape (13), single user mag tape (2), single user disk (15), terminal I/O host (7), multi-user tape (1), multi-user DOS (4), background/foreground (5), multi-user plus batch (2). However, concerning the use of high level languages, it is clear that Fortran (21 users) and Basic (15) are the most widely used.

Finally, a series of questions was included to determine the number and type of courses presently being offered in the real-time area. Twenty-four (of 48) departments indicated that one or more courses which utilize real-time computing in a supportive manner are being taught. Thirteen departments are teaching courses directly concerned with real-time computing. Nine departments offer real-time courses jointly with other departments. Sixteen departments have their students obtain real-time instruction from other departments. And four departments actually provide service courses for use by majors in other departments including computer science.

In summary, real-time systems and instruction in real-time computing no longer are novelties within the chemical engineering field. With the further decrease in hardware prices resulting from microprocessor applications we can expect total coverage of departments within the next several years.

FORTRAN DEVELOPMENT NEWSLETTER AVAILABLE

SIGPLAN (Association for Computing Machinery Special Interest Group on Programming Languages) Executive Committee has authorized the appointment of an ad hoc committee to take further steps toward formalization of a SIGPLAN Technical Committee on Fortran Development.

The purposes of the committee include: To form a bridge between active implementations of Fortran extensions and the ANSI X3J3 Fortran standards effort. To provide a forum for interchange of ideas and proposals, for groups interested in extending the Fortran language in various ways. To obtain and distribute information concerning developments in, and extensions to, the Fortran language as defined by existing standards. To take stands and make recommendations (after adequate consultation with all interested parties) concerning the desirability or undesirability of implementing certain features in certain ways, in the hope of reducing the proliferation of dialects by reacting in a timely way to new language developments.

The Fortran Development Newsletter, called FOR-WORD, is an informal publication of the SIGPLAN Ad Hoc Committee on Fortran Development. Information concerning the committee and its purposes is available from the Newsletter. Issues of the Newsletter distributed between February 1975 and January 1976 have been collected into a single volume in report form. Requests for additions to the mailing list and for previous editions (ask for FOR-WORD, Volume 1) should be directed to the Editor:

Loren P. Meissner
50-B 3239
Lawrence Berkeley Laboratory
Bekeley, CA 94720

COMING EVENTS

Atlantic City AIChE Meeting (Aug. 29-Sept. 1, 1976)

Process Synthesis: Research and Applications (2 Sessions). The sessions will be in the poster format, and will include discussion of such topics as reaction path synthesis, reactor systems, distillation system synthesis, energy recovery networks, and the synthesis of complete processes. Session Co-Chairmen: G. J. Powers and A. W. Westberg

Chicago AIChE Meeting (Nov. 28-Dec. 2, 1976)

Advances in Chemical Engineering Computing (2 Sessions). Session Co-Chairmen: D. G. Fisher and E. M. Rosen

Applied Mathematics in Chemical Engineering: Analytical Methods. Session Chairman: S. W. Churchill

Computers in Education: FLOWTRAN, APL, CAI, Minicomputers. This session will concentrate on new and innovative applications of computers in chemical engineering education. Session Co-Chairmen: Jude T. Sommerfeld and J. Peter Clark

Systems and Process Control (4 Sessions). These sessions will cover industrial applications, pilot plant studies and theoretical developments in process dynamics, systems, and process control. Session Co-Chairmen: J. D. Wright, D. Georgahis, and S. Marcikic

Other Meetings

National Computer Conference, June 7-10, 1976, New York City Summer Computer Simulation Conference, July 12-14, 1976, Washington, D.C.

Joint Automatic Control Conference, July 27-30, 1976, Purdue University, West Lafayette, Indiana

Second International Symposium on Computer Methods for Partial Differential Equations, June 22-24, 1977, Lehigh University, Bethlehem, Pa. Papers should be submitted to Prof. Robert Vichnevetsky, Department of Computer Science, Rutgers University, New Brunswick, N.J. 08903. Proceedings of the previous symposium contain 70 papers and are available at a cost of $29 from AICA, Department of Computer Science, Rutgers University, New Brunswick, N.J. 08903.

Short Courses and Workshops

Distillation Dynamics and Control, May 10-14, 1976, Lehigh University, Bethlehem, Pa. $350. In-depth study of the application of dynamic analysis and control techniques to distillation. Course organizer: W. L. Luyben

Process Design and Simulation with FLOWTRAN, July 6-9, 1976, University of Pennsylvania, Philadelphia, Pa. 125. Contact Mr. H. I. Abramson, AIChE.

New Developments in Modeling, Simulation and Optimization of Chemical Processes, July 26-August 4, 1976, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139. Presents basic principles and techniques for computer aided design and control of industrial-scale chemical processes. Contact Director of Summer Session, MIT, Room E19-356, Cambridge, Massachusetts 02139.

Computer-Aided Design of Chemical Processes, July 26-30, 1976, Northwestern University, Evanston, Illinois 60201. Brochures on study outline and objectives available from Continuing Engineering Studies, 2804 Technological Institute, Northwestern University, Evanston, Illinois 60201. Telephone (312) 492-3365.