

# AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

NEWSLETTER OF THE COMPUTING AND SYSTEMS TECHNOLOGY DIVISION - FIRST QUARTER 1978

Sigmund J. Lawrence - publications chairman  
Rodolphe L. Motard - feature editor  
Edward Gordon - feature editor  
Joseph F. Zemaitis, Jr. - reviews editor

This issue of the newsletter is the last put together solely by the editor. Future issues will involve the group listed above, and others as time and fate evolve. To the CAST division, the most important event at this time is the election of the officers. At the time of this writing, the election is still underway. However, as soon as the voting is closed and the votes counted, Bob Morris is to phone Sig Lawrence, and the results will be inserted as a flash bulletin elsewhere in this issue. Look for it. A history of the beginnings as the Machine Computation Committee and its metamorphosis into the Computing and Systems Technology Division is also presented in this issue. The feature article is on ASPEN (Advanced System for Process Engineering), a software project to meet the needs of the 1980's.

## CAST PROGRAMMING BOARD

The objectives of the Division, as related to programming are stated as follows: "to further the application of mathematical and computing principles in all aspects of chemical engineering especially in analysis, design, and control of process and management systems;" and "to exchange nonconfidential information concerning all facets of mathematics, management science, computers, control, and systems activity through meetings, seminars, courses, and publications."

Based on this charter, the Programming Board has responsibility to provide programming at the AIChE meetings and in continuing education courses to carry out the Division objectives. The Board will be headed by a chairman and backed up by a first and second vice chairmen and sections within the Board which will program in specific areas related to the overall objectives. At the present time, the new Division will absorb the activities of the former programming areas within the

National Programming Committee of: 1d) Applied Mathematics and Information Processing, 2L) Systems and Process Control, and 5c) Management Science. However, in the latter two cases, there will be a potential split between the Division programming and the National Program Committee areas. In both cases, the application side of systems and process control and management science techniques will remain with Group 2 - Unit Operations and Process Equipment and Group 5 - Management, respectively. Initially, our programming will remain essentially the same as it has been within the Machine Computation Committee and the three areas in the National Programming Committee that I have mentioned. However, since the scope of our activities can be redefined at this time, we are looking at what would make sense for the Division versus the Committee and Program Committee activities in the past. Some time within the next three months, we are going to rewrite our "charter" for programming in the new Division. I sincerely solicit any suggestions or thoughts that the membership might have in this regard. You can contact me by letter or by phone as follows:

Dr. Fred C. Stults  
PP&R Department  
Du Pont Company  
Wilmington, Del. 19898

Phone: (302)-774-8748

## SURVEY ON INTEREST IN MACHINE COMPUTATION

The MCC sent approximately 2,000 questionnaires to AIChE members involved with or interested in machine computation. Responses numbered 684 and all those received by Aug. 1, 1977 are included in the summary of the report below. This response is a great expansion of the 70 responses received in 1975 and should be more representative. The 1977 questionnaire was changed from the 1975 version and included a comprehensive question on programming languages.

The respondents to the 1977 survey represent a broad section of interest in machine computation. In contrast to the 1975 survey, which had about half its respondents from academic institutions and engineering design, construction or consulting firms, the 1977

(See page 3  
for Luncheon)



respondents were more representative of the major industries - chemical, petroleum refining, petroleum and petrochemicals (40 percent of respondents). Academic institutions accounted for 11.7 percent and engineering design, construction or consulting firms for 11.4 percent.

Conclusions which can be drawn from the questionnaire are:

- The majority of the respondents (87.5 percent) are chemical engineers
- FORTRAN is used by about 70 percent of the respondents as compared to 81 percent in 1975
- IBM machines are used by 44 percent (54.2 in 1975)
- Twice as many respondents use in-house process simulation programs than use the commercially available programs
- GPSS (General Purpose System Simulator, IBM) is the most popular choice of a discrete system simulation program (38 percent of program users)
- CSMP (Control System Model Program, IBM) is the most popular choice for continuous system simulation (46 percent of program users)
- There is a high level of interest in learning about the simulation languages (57 percent of all respondents)
- The level of interest in MCC is high with 150 respondents interested in joining

-by Calvin B. Cobb

#### CORRECTION

In the last issue of the newsletter, the correct place to obtain Volumes I and II of "Introduction to Microcomputers" is: Newman Computer Exchange, Inc., 1250 N. Main, Ann Arbor, Michigan 48104.

#### OBITUARY - ALBIN I. JOHNSON

Albin I. Johnson, Dean of the Faculty of Engineering at the University of Western Ontario in Canada, died on October 8, 1977 at the age of 53. "Ab" was a member of the Machine Computation Committee. For more than 2½ decades at four universities he initiated projects to attract outstanding students to the engineering profession. Many who crossed paths with him referred to A.I. as "AB the Avid Initiator". A few weeks before he died he learned at a public ceremony that a start had been made to establish the A.I. Johnson Scholarship for undergraduate students at Western. This news gave him great comfort and helped to sustain his spirits during his final days. His extemporaneous remarks made in acknowledging this award resulted in a standing ovation.

A minimum of \$25,000 is deemed essential to fund an attractive entrance scholarship in Engineering Science. If you are interested in supporting this cause, send your check, (tax deductible) payable to The University of Western Ontario, A.I. Johnson Scholarship Fund and forward to the Office of the Dean, Faculty of Engineering Science, The University of Western Ontario, N6A,5B9. This information was furnished by J.E. Zajic, chairman of the scholarship committee.

#### COOPERATIVE PHYSICAL PROPERTY DATA PROJECT

By request from interested chemical industry representatives, a committee has been appointed to study the formation of a Design Institute for Physical Property Data (DIPPR) under AIChE auspices. This cooperative program would compile component data, measure missing pure component properties, encourage phase equilibrium correlation and prediction efforts, and measure mixture properties for selected systems. The purpose of this program is to serve the data needs of the chemical industry in satisfying environmental, safety, and energy conservation requirements, and in reducing duplication of effort in obtaining data.

It is envisioned that specific projects would be separately funded by interested companies and contracted to various investigators. Central to the program would be a Data Compilation Project, and other projects would contribute to it.

John Prados, University of Tennessee, has been named chairman of the committee. Contact him at 705 Andy Holt Tower, Knoxville, Tenn. 37916. (Phone (615) 974-3211) for additional information.

-by A. H. Larsen

### DELPHI LOOK AT "COMPUTING IN THE 1980s"

T.I. Peterson, IBM Corp., Armonk, NY  
M.T. Tayyabkhan, Mobil Research and Development Corp., Princeton, NJ

This is the second of a three-part series. The first part appeared in the previous Newsletter.

What's ahead for computing and its impact on chemical engineering? That's the topic that was directed to a panel of experts in The Second Pacific Chemical Engineering Congress (Pachec '77), Denver, Col., Aug. 28-31, 1977.

In the last issue of the Newsletter, Sig Lawrence reported on the questionnaire which constituted Round 1 of the Delphi Study. Now, we turn to an analysis of the responses which formed Round 2 and provided the basis for Round 3, the panel discussion.

Details of the questionnaire and the responses will be found in the Proceedings of Pachec '77, Vol. II, pp. 830-842. Here, we summarize the results.

The questions, 71 in all, covered a wide range of computer involvement. They were distributed as follows: computing-19, hardware-10, process control-5, general DP applications-5, micros-5, data bases and communications-5, input/output-5, distributed computing-4, software/firmware-3, chemistry applications-2, education-2, privacy-2, and one each for chemical engineering design applications, reliability, regulation and management.

The responses came from two groups. Queries were sent to 144 chemical engineers and 125 computer scientists. Bonafide replies were received from 67 engineers and 32 scientists. Of the engineers, 26 were academic, 34 were industrial and 7 other. All of the scientists were academic.

Conclusions which were more certain include: Centralized computing will become more specialized. There will be a relatively rapid movement to distributed computing. Micros and minis will abound fairly quickly. There will be a continued reduction in the price/performance ratio. There will be a prominent role for the end user. Some problems, such as leaks and fraud, will never be solved. Technology will continue to progress. Computing will always be judged with a price tag. The emphasis will be on software and applications productivity. Computer use will become routine throughout education. Business will integrate more closely with computers. Computing utilities will become regulated.

Conclusions which were less certain include: Total hardware cost in installation constant? Programming a persistent bottleneck? When acceptable methodology for distributed DB's, computing networks? Solution to problems of installability, reliability, DP impact measure, programming accountability, training? Automated reaction syntheses? NRCC (National Resources for Computation in Chemistry) objectives met? New applications systems satisfy needs of process engineers? Rate of growth of office automation, text processing? Rate of progress in secondary storage? When graphics input? How rapid miniaturization? When consumer-based computer products? True man-computer symbiosis?

PACHEC '77 saw some heated discussion about those "Less Certain" areas. Look into the next newsletter for more on that colloquy.

### ANNOUNCEMENT OF CAST DIVISION LUNCH & MEETING

The executive committee of the Computing & Systems Technology Division will meet in Atlanta, Georgia, on Monday, February 27 from 2-5 pm in Tower Suite 12 at the Peachtree Plaza Hotel. Division members are invited to attend. The meeting will be preceded by an informal luncheon for members of the division. The menu will be baked chicken, with appetizer, beverage and dessert. The cost is \$8.25 including taxes and gratuity. Send your reservation and check, payable to "CAST Division AICHE" to Charles H. Ware, Jr., Commercialization Insights, 33 Sandi Drive, Poughkeepsie, NY 12603. Lunch reservations must be made by Feb 17. This will be the only announcement of the luncheon.

CACHE (COMPUTER AIDS IN CHEMICAL  
ENGINEERING EDUCATION)

At its sixteenth biannual meeting in August, 1977 the Board of Trustees of the CACHE Corporation added three industrial members: Edward Rosen (Monsanto), Ted Leininger (DuPont) and Louis Tichacek (Shell). Current officers of CACHE are: Duncan Mellichamp (UC Santa Barbara), President; David Himmelblau (Texas-Austin), Vice-President; R. L. Motard (Houston) Secretary and Lawrence Evans (MIT), Executive Officer. The trustees are, in addition to the above: Carnahan (Michigan), Edgar (Texas-Austin), Fogler (Michigan), Henley (Houston), Hughes (Wisconsin), Mah (Northwestern), Ramirez (Colorado), Seader (Utah), Seider (Pennsylvania), Smith (LSU), Stephanopoulos (Minnesota), Weaver (Tulane), Westerberg (Carnegie-Mellon), Jim White (Arizona), Wright (McMaster).

Recently, eight introductory monographs on Real Time Computing have been completed. The fourth monograph is now in print and the complete set will be available in March, 1978. These may be ordered from Professor Brice Carnahan, Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan 48109 for \$20.00 for the full set.

The ChEMI project (Henley) reported that 150 of the approximately 350 scheduled instructional modules in seven basic chemical engineering subject areas are ready for publication and distribution. Arrangements for publication will be announced shortly; however, it now appears that AIChE may be the publisher on the basis of recent actions by the AIChE Continuing Education and Executive Committees.

The Large Scale Systems and Program Distribution Task Forces are continuing to support the successful FLOWTRAN project. The program is made available at cost to departments of chemical engineering by a commercial service bureau. Over 35 schools have used this service in three years. A review of national/international network services is underway to reduce the cost to the users and to expand the number of programs to be offered. Some twelve to fifteen programs have been identified as potentially useful in educational projects. These programs originate in U.S. and European universities and range from process synthesis packages

to computer supported instruction. The FLOWTRAN project will be publishing a new User's Manual and a casebook of FLOWTRAN exercises collected by J. Peter Clark (Virginia Poly).

CACHE Vice-President Himmelblau is heading an effort to define the role of CACHE in its second decade. Three major factors are impacting our activities as educators:

(1) Technologies of Communication and Dissemination.

These new technologies seem ready to be integrated into the educational process, including: inexpensive computers, electronic communications, large data networks, central data banks, revolutions in printing and display, video disc and cassettes and personal computers.

(2) Changes in the Instructional Process.

Many of the technological innovations mentioned above will cause an evolution in the characteristics of: texts, instructional modes, techniques of engineering analysis and synthesis, laboratory experiences and continuing education.

(3) Societal Constraints.

Any plan for the future must reflect a new found awareness to the issues confronting society such as: energy, safety and reliability, toxicity of materials and products, waste disposal and environmental control, materials substitution, complexity of society, population demographics and profits and productivity.

All of these issues have implications related to a needs assessment of the chemical engineering curriculum. Technological innovations introduce constraints as well as provide opportunities.

-by Rudy Motard

## AICHE AREA 15a - PROPOSED SESSIONS

The following 11 AIChE meeting technical sessions have been proposed by the Applied Mathematics and Information Processing subcommittee (formerly Area 1d) for 1979. The chairmen indicated by an asterisk are only proposed and must yet agree to participate. One session, that entitled "Process Synthesis Methodology - A Critical Review" to be held in Boston, will comprise a solicited pair of review papers followed by a panel discussion.

-by Art Westerberg

### Houston - April 1979

Optimal Allocation in Energy Networks

R. Pike, F. Pitts

Simulation of Fossil Fuel Related Processes

L. Evans\*, L. Joseph\*

Sparse Matrix Computational Methods

R. Mah, A. Westerberg

### Boston - August 1979

Finite Element Methods

B. Finlayson\*, S. Churchill\*

Process Synthesis Methodology - A Critical Evaluation

H. Null\*, J. Siirola\*

Computers in Education and Training

G. Marr\*

### San Francisco - November 1979

Computers in Design and Control  
(2 sessions)

J. Douglas\*, E. Rosen

Applied Mathematics in Chemical Engineering

W. Schiesser\*, J. Seinfeld\*

Personal Computing

M. Tayyabkhan

Free Forum in Computer Technology

G. Stephanopoulos\*

## CALL FOR PAPERS

### Symposium on Impact of New Developments in Computer Hardware & Software

Two Sessions

AIChE 71st Annual Meeting

Miami, November 12-16, 1978

Chairman

Professor Richard S. H. Mah

Department of Chemical Engineering

Northwestern University

Evanston, IL 60201

Co-Chairman

Dr. C. Dwight Prater

Mobil Research and Development Corporation

Paulsboro, NJ 08066

Papers on the following topics are solicited:

1. Application of microprocessor technology, computer graphics, and programmable calculators
2. Application of data based systems in integrated process and project engineering
3. Generalizable experience on and evaluation of computer networks and parallel processors
4. Impact of new programming language and software on chemical engineering problem-solving

Proposal-to-Present Form should reach Chairman by March 1, 1978.

Final manuscript should reach Chairman by June 15, 1978.

### BYTES AND PICOS (BITS AND PIECES)

At the National Meeting in Philadelphia during early June, 1978, the First Chemical Plant Equipment Exposition will be held. Bob Fisher of CAST is preparing a tour guide directed at booths of interest in computing and systems technology. Such will help you get thru the maze.

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Never insult an alligator until you have crossed the swamp.

## HISTORY OF FORMATION OF CAST

At the Denver meeting in August, Council formally approved the formation of the Computer and Systems Technology Division. C&ST will begin operating formally in January, 1978. The objectives of this division are:

- a. To further the application of mathematical and computing principles in all aspects of chemical engineering, especially in the analysis, design and control of process and management systems.
- b. To recommend to the Council of the AIChE positions or policies related to such applications.
- c. To provide suitable programs to inform Institute members about topics of current interest in these fields.
- d. To provide a communication medium for chemical engineers and other individuals to exchange nonconfidential information concerning all facets of mathematics, management science, computers, control and systems activity through meetings, seminars, courses and publications.
- e. To coordinate the Institute's activities with other societies active in this field.
- f. To act as a source of information for chemical engineers who are not actively engaged in the mathematics, management, computer, control or systems fields, and to bring to their attention the importance of these activities, the need for consideration of their use in the general practice of chemical engineering and opportunities for their use in research, development, design and operation of process and management systems.
- g. To encourage chemical engineering educators to place suitable emphasis on these subjects and encourage excellence in such teaching practices.

This new division has its roots in the Machine Computations Committee. In June 1974, Charles Ware reported on MCC activities to Council. One council member suggested that the scope of the activities indicated the advisability of the formation of a division. A subcommittee, headed by Robert Morris, with Oran Culberson, Herb Owens and Mike Tayyabkhan, was formed to prepare a specific proposal to the MCC at the Kansas City meeting in 1976. This proposal included: establish a division formation committee; draft division by-laws; solicit selected AIChE members for potential interest; prepare an operating plan and budget; and select a name for the division.

In August, 1976, Al Caselli, Council liaison, notified Council of MCC's plans to organize a division. By this time over 500 AIChE members had supported division formation, including 75% of Area 2L members.

The Division Formation Committee met for the first time in November 1976. It consisted of Bob Morris, chairman, with Brice Carnahan, Mary Ann Epstein, Bob Fisher, Dick Hughes, Al Johnson, Max Lee, Ted Leininger, Dick Mah, Herb Owens, Ted Peterson, Manoj Sanghvi, Warren Seider, Vern Sterba, Charlie Ware, Bob Weaver and Art Westerberg. Fisher led the By-Laws subcommittee. Seider prepared the budget. Sterba and Ware prepared the operating plan. The DFC did its work properly and several presentations were made to Council.

Since Council's formal approval at Denver, a nominating committee and an executive committee were formed. Bob Morris heads both committees. Candidates for the division offices were nominated and the election got under way. Only those who have paid C&ST Division dues were eligible to vote. The nominating committee included Mack Clark, Bob Fisher, Dick Hughes,

Sig Lawrence, Bob Morris, Mike Tayyabkhan, Charlie Ware.

The executive committee includes: Brice Carnahan, Al Caselli, Mary Ann Epstein, Bob Fisher, Bob Harris, Al Johnson, Bob Lackmeyer, Sig Lawrence, Max Lee, Ted Leininger, Dick Mah, Herb Owens, Ted Peterson, Manoj Sanghvi, Warren Seider, Vern Sterba, Fred Stults, Mike Tayyabkhan, Charlie Ware, Bob Weaver, and Art Westerberg.

Members of the AIChE who are interested in joining the division should contact Bob Lackmeyer, Acting Treasurer, Standard Oil of Ohio, Midland Bldg-215CB, Cleveland, Ohio 44115; phone (216)-575-5002.

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#### ASPEN PROJECT UPDATE - Feature Article by L. B. Evans and P. W. Gallier

ASPEN is a major, new process simulator for engineering fossil fuel conversion processes. As an "Advanced System for Process Engineering" this simulator is aimed at helping the U.S. Department of Energy (DOE) to do a better and more efficient job of getting fossil fuel conversion plants into place.

With the need of the U.S. to find alternative energy sources to oil and gas for the future, the DOE sees large expenditures needed for fossil energy process development. Tough decisions will have to be made between alternative processes. Tradeoffs must be analyzed involving process technology and economics. The ASPEN system is intended to help in providing a rapid, analytical tool which would permit a consistent means of evaluating these processes.

Under development at MIT, the ASPEN system is to have new capabilities to model process operations found in conversion plants, such as coal handling and coal conversion reactors, as well as conventional vapor-liquid processing. The system is being designed to be flexible to allow variable types of streams and to allow insertion of specific, even proprietary, process models. A key feature will be its ability to estimate plant costs and to make economic analyses for plant investment.

Funded by DOE at \$3,285,000 for three years, the project is now into its second year and well underway. The principal investigator is Prof. Lawrence B. Evans at MIT. The Project Manager, Dr. Paul W. Gallier, is on loan from Monsanto Co. The principal staff is composed of nine people with industrial experience and some in post-doctoral positions. They are assisted by a large number of MIT students who are working on the Project. At DOE, the Project Manager is Dr. Carlos W. DiBella. Part of the work is being done at the University of Pennsylvania under a subcontract to co-investigator Professor Warren D. Seider.

#### Functional Specifications

Recent work on the project has been to complete a document detailing the functional specifications of ASPEN. These are the functions ASPEN will perform without dealing with how they will be done. A summary of these specifications is made here.

ASPEN will be capable of providing detailed heat and material balances and detailed economic analyses for process plant construction and operations. ASPEN will provide an extensive data base for coal physical properties, routines for solids handling, and routines for waste product recovery systems.

Building-block subroutines will be developed to model all of the common unit operations in fossil energy processes. About seventy-five unit operations models are planned. These include stream addition, steam splitters, distillation column, adsorption columns, extraction units, pumps, compressors, expanders, turbines, equilibrium flashes, heat exchangers, heaters/coolers, condensers, furnaces, cyclone separators, crushers, grinders, screens, kilns, fluidized bed heat exchangers, filters, centrifuges, driers, electrostatic precipitators, and crystallizers.

Subprograms will be included to model standard reactor types such as the equilibrium reactor, well-mixed reactor, homogeneous tubular reactor, catalytic fixed-bed and fluidized-bed reactors. Where models exist of specific reactors involved in fossil fuel conversion processes (such as gasifiers, liquefaction reactors, oil-shale retorts, etc.) they will be programmed and included in the system. Programs will be provided to model the major process units for sulfur recovery (such as the Claus reactor, amine scrubbers, etc.).

The best available algorithms for convergence of recycle streams will be implemented. There will be provision for automatically adjusting process equipment parameters to achieve specified values of stream variables for the purpose of design of processes.

A variety of options will be provided for computing physical properties (different equations for vapor pressure, equations of state, activity coefficients, etc.) and it will be possible for the user to specify the computational method to be used. The user may also add new physical properties and their methods of computations. Default options will be available for the user who prefers to use standard methods.

The available property models will represent the state of the art in equations of state, corresponding states correlations, activity coefficient models, and other types of correlations. New models may be readily added to the system by the user.

The data banks provided as part of ASPEN will contain a comprehensive set of physical property constants for the vapor, liquid and solid phases of pure compounds, the important properties of a number of standard types of coal, and the parameters of certain classes of property correlations for both pure compounds and coal. The property subsystem will be designed to readily accommodate additional data banks provided by the user. All of the data banks will be accessible by the simulator executive system and the physical property subsystems.

A data regression subsystem will allow the user to supply information in the form of raw data from which property constants and/or correlation parameters are determined by linear or non-linear regression. The user may specify which models are to be employed for this, and which constants and/or parameters are to be treated as regression variables. The results may be placed in an output file or stored directly in one of the data banks.

Equipment sizing and costing calculations will retrieve information from data banks and the heat and material balance calculations. Two levels of accuracy for cost estimations will be possible. These are: (1) an order of magnitude estimate for screening and process studies and (2) a study estimate ( $\sim 30\%$ ) based on knowledge of major items of equipment.

In addition various types of economic analysis will be possible for the process model. These include: capital investment, operating costs, profitability, and sensitivity analysis.

### Special Features

Most process simulators used in industry today employ the sequential modular method of computation. This is based on the concept of calculating outputs of a unit given the input streams and parameters. The decision made for ASPEN is to use this computational architecture but with some advanced, optional assists. By deciding on this as the basic computational structure, ASPEN can take advantage of a wide range of available unit operation routines and also allow simpler addition of new routines. The assists will be in the form of (optional) automatic tear stream selections for recycle loops, and automatic definition of the best computational sequences.

State-of-the-art and improved convergence methods and control capability (to meet design requirements) will be provided.



Another option planned to be implemented is simultaneous modular computation. This method promises a speed advantage for complex recycle processes and for meeting design specifications. It combines a solution of the flowsheet by linear models along with the rigorous models of the sequential modular method.

### Structured Design

The ideas of structured design and structured programs are being implemented fully in the ASPEN Project. These methodologies are being adapted with the help of SofTech, a software engineering firm nearby in Waltham, Mass. The structured design methodology proposed by Myers and Constantine in 1975 promotes good staff interaction in design and eliminates expensive errors (of logic and structure) in the early stage of the project. The methodology should result in modular code with an improved maintenance factor.

### Advisory Committee

Liaison with a wide variety of industrial users is being kept during the Project through an ASPEN Advisory Committee. About 60 different individuals from 40 different companies serve to review and advise the Project's progress. The next meeting of the Advisory Committee was January 9-10, 1978 at M.I.T. This makes us feel somewhat like "working in a goldfish bowl", but the advice obtained for developing a desirable product is highly necessary.

### Schedule

The overall Project is scheduled for completion in September, 1979. Some milestones indicating the completion of phases of work can be outlined as

<u>Phase</u>	<u>Completion Date</u>
1. Staffing, Surveying Programs, and Design Criteria	November, 1977
2. Design of Executive and Subsystems	April, 1978
3. Implementing Basic System	September, 1978
4. Implementing Complete Systems and Testing, Documenting Basic System	April, 1979
5. Test and Document Complete System	September, 1979

A critical path planning and control program, PROJACS, is being used to schedule the more than 250 different activities of ASPEN.

One might say, "Schedules, like promises, are made to be broken". The ASPEN Project team is committed to this schedule, but above all, the Project is committed to producing a quality process simulator for widespread usage for DOE.

## EDITORIAL - THE MEANING OF LIFE

The death of Ab Johnson, member of the Machine Computation Committee, is met with both sorrow and hope; as it should be when friends or relatives pass away. An obit appears elsewhere in this issue. This event provides the proper motivation for me to discourse on the meaning of life.

To every living thing, death is inevitable; taxes to most humans; and in the words of Jerry Coe, spoken twenty years ago: "instrument maintenance" to many. I am not a guru in the accepted sense of the word. But I have developed a philosophy of life through diligent search, an open mind and a good analytical training as a chemical engineer. Please consider the following as a series of questions to think about. Engineering is a means of earning a living, but it has nothing to do with the meaning of life. In one sentence, our purpose in life should be to perfect ourselves to such a point that God can manifest in each of us as an individual. But, what is that perfection? Not that we stop making mistakes, which might hurt others. Rather, that as soon as we recognize that we have affected others, we immediately correct and atone for that error. Also, to love all creation.

Further, if you have been around as long as I have, 59 years, you realize that there hasn't been much improvement in this lifetime. Therefore, it must take many lifetimes to make any significant amount of improvement. So we come back again and again in the inexorable helix of life, hopefully rising higher on the spiral with each experience.

The present is an infinitesimal instant between the past and the future. The past stretches back for eons to when we were created. The future stretches into eternity. Though we live and operate in the present, for all intents and purposes we are in eternity right now. Therefore, let us face each moment with our eternal goal ever in mind, oneness with God. To achieve this, we must love God, only the one God, and love our neighbor as ourselves.

## FLASH - ELECTION RESULTS!!!

The first election for officers of the brand new Computing & Systems Technology Division has been completed. The results are summarized below.

A total of 76 valid ballots were received by December 21, with postmarks of December 15, or earlier. The official count of votes for the winners is as follows:

Chairman	V. J. Sterba	76
1st Vice Chairman	W. D. Seider	75
2nd Vice Chairman	R. E. Weaver	41
Secy. - Treasurer	R. J. Fisher	39

Directors:		
1978-1980	M. T. Tayyabkhan	59
	T. I. Peterson	54
1978-1979	R. R. Hughes	49
	R. L. Morris	46
1978	R. L. Motard	46
	P. L. Gallier	43

We congratulate the elected. With your support for the new officers, the CAST Division shall rise from its embryo, the Machine Computations Committee.

## NRCC

The National Resource for Computation in Chemistry will become a division of the Lawrence Berkeley Laboratory. NRCC will use LBL's existing computing center which has a Control Data CDC 7600 computer coupled with two CDC 6000 series computers. (C & EN, Aug. 22, 1977).

The NRCC staff will be able to document, test and improve software; develop new computational methods; design specialized hardware and software particularly suited to solving chemical problems, and conduct chemical and computational research.

The comforting thought is that the reliability of chemical data obtained by theoretical methods appears to be competitive with that of data obtained from experimental sources. (C & EN, Sept. 12, 1977)

SIGNUM - SPECIAL INTEREST GROUP ON  
NUMERICAL MATHEMATICS CONFERENCE CALENDAR

<u>Date and Title</u>	<u>Place/Sponsor/Contact</u>
March 15-17, 1978 Eleventh Annual Simulation Symposium	Tampa, Florida SIGSIM, IEEE-CS, SCS Ira M. Kay Box 22621 Tampa, Florida 33622
March 29-31, 1978 1978 Mathematical Software Meeting	Austin, Texas C. S. Dept., Center for Numerical Analysis A. Sherman Computer Sciences Department University of Texas Austin, Texas 78712
May 26, 1978 Computer Algebra Symposium	Madison, Wisconsin SIGSAM in cooperation with SIAM G. E. Collins Computer Sciences Dept. University of Wisconsin Madison, Wisconsin 53706
June 1-3, 1978 Conference on History of Programming Languages	Los Angeles, California SIGPLAN B. G. Claybrook Computer Science Dept. VPI Blacksburg, Virginia 24061
Aug. 28-Sept. 1, 1978 Eighth Australian Computer Conference	Canberra, Australia Australian Computer Soc., Inc. ACS-8 Programme Committee P.O. Box 448 Canberra, A. C. T. 2601 Australia
Oct. 30-Nov. 1, 1978 Symposium on Future Trends in Compute- rized Structural Analysis and Synthesis	Washington, D. C. University of Maryland George Washington University NASA-Langley Res. Center Ahmed K. Noor Mail Stop 246 NASA Langley Res. Center Hampton, Virginia 23665

KOPTYUG VIS A VIS LYKOS

C & EN (Nov. 28, 1977) reports that Dr. Valentin A. Koptuyug of the Soviet Academy of Services, spent nearly a week of his October month-long visit to the USA conferring with Dr. Peter G. Lykos of Illinois Institute of Technology about the upcoming Fourth International Conference on Computers in Chemistry and Chemical Education. This will be held in Novosibirsk next June and hosted by the Siberian Institute of Organic Chemistry at Academy Town, outside Novosibirsk.

Koptuyug credits Lykos with much of the initial work to bring this conference, which in the past has been a conference primarily of western computer chemists, to the USSR.

Peter Lykos wrote about this conference in our newsletter for the first quarter of 1977. He was 1977 chairman of COMP (Computers in Chemistry, a division of ACS).

Recently, Peter organized the mailing of a survey to determine user needs for the very large scientific computer systems that might become available in the next decade.

Conducted by NASA and IIT, the survey is aimed at computers about 100 times more powerful than current machines-handling about 10 billion instructions per second. Problems such as modeling the earth's climate or the U.S. economy, cracking complex codes, or analyzing nuclear reactions might be studied. The needs of a multinational corporation, or food and shelter for the peoples of the world might be studied.