Computing and Systems Technology Division Communications

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News and Information

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About This Issue

Peter R. Rony and J.D. Wright

This is the fourth issue of CAST Communications since we assumed editorial responsibility in the Spring of 1985. The following pattern should now be evident in the newsletter:

(a) A strong emphasis on our Meetings and Conferences section, with listings as far into the future as are available. As discussed by CAST Director Bruce Finlayson in this issue, such listings permit CAST Division members to plan in advance their presentations and publications. We thank members of the CAST Programming Committee for their diligence in supplying this information.

(b) Enhanced communications between members of the CAST Division Executive Committee and CAST Division members. Communications consist of messages from the CAST Division chairman, awards committee chairman, program committee chairman, editor of the newsletter, and other officers. The CAST officers serve you, and it is important that you know what is happening in the Division.

(c) One, or sometimes two, feature articles on a timely subject of potential interest to CAST Division members. We do not copyright the CAST Newsletter, so publication of such an article does not preclude its publication in a scholarly journal or magazine. You may have observed that George Stephanopoulos protected his author's rights by copyrighting his article, "Expert Systems and Computing Environments for Process Systems Engineering," in Volume 9, No. 1 (June 1986). If such a practice helps the CAST Newsletter obtain better articles, we are delighted. We thank all of our feature article authors

for their confidence in and support of the newsletter.

(d) Reports from various groups—CACHE, DOE Workshops, Engineering Research Centers, and so forth–that bear on current plans and activities in the computers and systems technology area. Again, the goal is to enhance communications among professionals in the chemical engineering computing community.

(e) A new tradition–published excerpts from the award lecture given at the fall CAST banquet by the Computing in Chemical Engineering Award winner.

(f) A newsletter that has greater texture and a more standard publication style. This has been through the efforts of Associate Editor Joe Wright and his capable secretaries, who have access to the Xerox 8010 Star at the Xerox Research Centre of Canada.

(g) Enhanced interaction between the newsletter editors and the CAST officers concerning what can and should be published in the newsletter. For this issue, our special thanks go to Chairman, Tom Edgar, who recommended the publication of the DOE Workshop excerpts, information on the winner of the Eckman award, and information on the Engineering Research Centers; Bruce Finlayson, who contributed a brief article on how to get a paper accepted for presentation at an AIChE meeting; W. MacMaster Clarke, who provided information on the 1986 CAST Division award winners; and Jeff Siirola and Rex Reklaitis, for their very detailed information on Area 10a session and FOCAPO plans.

Two other patterns that may or may not be so evident are:

(h) An increasing use of submitted articles and messages on IBM PC format

floppy disks. The chairman's message, article on NASA/Goddard's massively parallel computer, and article on submitting a paper for presentation at an AIChE meeting all were provided to the editors on disks. A fourth contribution arrived on a MacIntosh 3.5" disk, but we did not have access to a Macintosh-to-IBM PC communications link (nor knowledge of how to use the Macintosh). You can appreciate how helpful such disks are for the editorial process. Your friendly editor (or his secretary) must retype any newsletter information that is received in manuscript form–a waste of time, in our opinion. We encourage the AIChE and the entire chemical engineering community to move toward the submission of text material in disk format, a form of enhanced productivity that is needed in a society where professionals are overloaded with work.

(i) Two missed publication deadlines. Our goal for each issue is publication one or two weeks prior to the AIChE meeting. Each issue requires about one man-week of concentrated effort by each of the editors (and their respective secretaries, if available). One editor organizes the issue, types and edits all contributions, and updates the Meetings and Conferences section. He then sends the material in electronic form (either by electronic mail or, in the case of this issue, by IBM PC format disks) to the other editor, who formats the entire issue, checks it for errors, and prints it in camera-ready form on a laser printer. The camera-ready copy is then sent to the AIChE offices, which print and mail the newsletter to CAST Division members within several weeks. Missed publication deadlines occur when timely windows to work on the newsletter are not available or disappear suddenly because of job demands on the volunteer editors.

What is in store for the 1987 issues of CAST Communications? Tom Edgar

has recommended an article or two on the subject of statistical process control. We have solicited contributions from Mark Stadtherr and other colleagues in the area of advanced computer architectures, including supercomputers. Finally, we hope to publish an article, originally scheduled for this issue but not yet received, on the Intel iPSC Multiprocessor (Caltech Cosmic Cube). We solicit suggestions from CAST Division members concerning other topics that would be of interest. We also wish to expand our editorial notes coverage to include items from CAST Division members abroad.

Any innovations for the CAST Newsletter in 1987? How about some humor, in the form of brief articles, spoofs, cartoons, or respectable jokes. CEP is notably devoid of humor, so perhaps the CAST newsletter can become the "patron saint" of chemical engineering humor. Since there may be a dearth of such material (we all give the impression of being such serious fellows), initially all types of ChE humor are invited, not just those that involve computing and systems technology in chemical engineering. Perhaps one day there will be an AIChE Humor in Chemical Engineering Award.

See you in Miami Beach.

Chairman's Message: Recent Trends in Chemical Engineering

Thomas F. Edgar, University of Texas

Hardly a day goes by when I do not read a newspaper or magazine article that discusses the interrelated themes of increased productivity, international competition, and high technology. The chemical and petroleum business is changing, whether we like it or not. As members

of a division within AIChE that is very much concerned with the frontiers of chemical engineering, we should be aware of several trends that have surfaced since 1984.
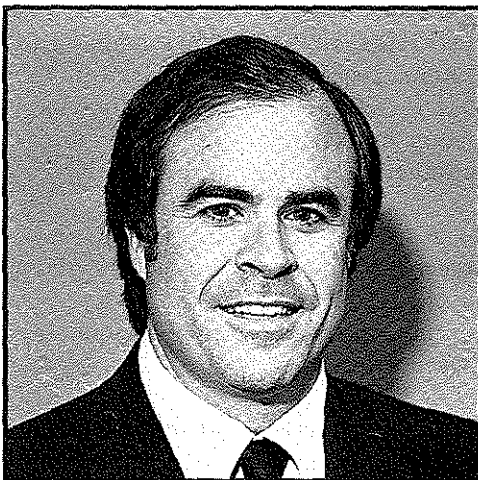
It is clear that industry has changed its emphasis from design of new facilities to increased efficiency of manufacturing. The trend toward manufacture of specialty products instead of commodity chemicals represents an effort to capture higher returns on investment and thus respond to increased international competition.

How will the increased emphasis on specialty chemicals affect members of the CAST Division? As pointed out by Jim Mathis, former Vice President of Science and Technology at Exxon (CEP, p. 19, July, 1986), these plants will

"call for more flexibility than continuous plants. They also require dynamic, not steady-state, control systems and batch systems optimization. At the same time, a hierarchy of control systems will be added for all plants on top of the local unit systems now in place. Raw material and product inventories can be precisely adjusted by having entire plant complexes linked and optimized on a real-time basis. The just-in-time

systems with these features will be introduced. Robots, automated vehicles, bar-coding, and other advanced materials handling technologies will be deployed. Local area networks will collect, store, and communicate all the information. Most maintenance will be done on-line when delicate sensors or databases containing all prior experience signal the need for it."

On the other hand, many plant managers may seek early retirement if their continuous processing plants are replaced by batch plants.

What about future employment trends? Many of us feel that the demand for computationally-trained chemical engineers will continue. However, this may be manifested in hiring more professionals with advanced degrees. In a recent thought-provoking paper at the Annual ASEE meeting, Dr. C. T. Sciance, Director of Engineering Research at Dupont, cited statistics for his company which show a doubling of Ph.D. hires in chemical engineering, while hiring of new B.S./M.S. graduates declined by more than 50%. Overall, the trend is toward hiring fewer chemical engineers who know more and who require less supervision. Dr. Sciance believes that computer technology is one of the educational areas where universities need much improvement, to enrich the teaching of all courses with computers and enhance student problem-solving skills. Finally, he points out that now is the time to revive the M.S. as the terminal degree for practicing chemical engineers (it has been 15 years since that idea was put to rest; I guess educational trends can have cycles just like the business sector). Certainly an M.S. degree would allow all students to become proficient in computing.

Obviously, all of these trends, if they reach maturity, will have a major

impact on both how we do things in education and industry and the supply and demand of chemical engineers. You ought to read the text of Dr. Sciance's lecture, which will be published in 1987 in **Chemical Engineering Education;** if you want a copy of the paper sooner, please write to Dr. C. T. Sciance at:

Engineering Department,
E. I. du Pont de Nemours,
ESL-304/229,
Wilmington, DE 19898

Memorial to Richard Robert Hughes

Warren E. Stewart, University of Wisconsin
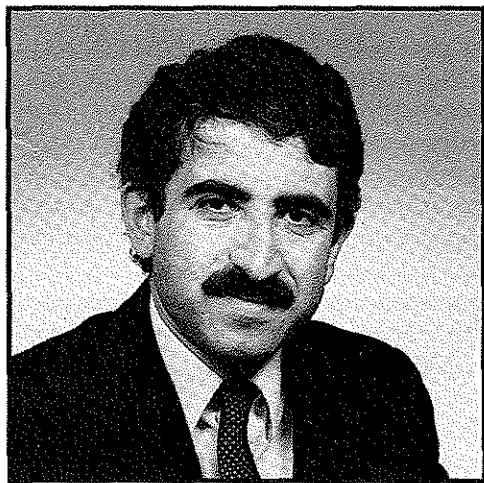
We report with sorrow the death of Professor Richard R. Hughes of the University of Wisconsin, Madison. Professor Hughes died June 16, 1986 in Bombay, India, where he was teaching a course on computer-aided design of chemical processes.

Dr. Hughes received his B.S., M.S., and Ph.D. degrees in Chemical Engineering from the Massachusetts Institute of Technology in 1942, 1947, and 1949. From 1942 to 1946 he served in the U.S. Army, participating

in the Mediterranean campaign and later as Instructor in Ordnance at West Point.

In his 19 years at Shell Development Company, Richard served in various management positions, including head of the Chemical Engineering Department. He returned to academia in 1968 as Professor of Chemical Enginering and Associate Director of the Engineering Experiment Station at UW-Madison.

Richard was a pioneer in applications of computers to chemical engineering at Shell, AIChE, and UW-Madison. He served as coordinator of computing activities at the University and as a charter member of the CACHE Corporation and the CAST Division. He was the founding editor of Computers and Chemical Engineering. He taught extensively on computer-aided design in the AIChE Continuing Education Program and, with his students, did important research on computer-aided design and optimization. These contributions were recognized in 1979 when he was named the first recipient of CAST's Computing in Chemical Engineering Award.

Richard served AIChE as a Director from 1969 to 1971, and as President in 1981. He was a Fellow of the Institute, and received a Founders Award in 1980. He served as Chairman of the CAST Division and the Continuing Education Committee, and Treasurer of the Environmental Division. He was a member of the committees on Education and Accreditation, Ethics, and New Technology.

Richard was well known for his community service. He sang with the Madison Symphony Chorus and Madison Opera, and was a supporter of many community organizations.

A memorial service for Richard Robert Hughes was held on August 10 in Madison, attended by his family and a

large company of colleagues and friends. Testimonies were given in appreciation of his devotion to his family, his students, his University, his community, and his profession. We express our appreciation here for his outstanding contributions to CAST and to AIChE.

Yaman Arkun Wins the AACC Eckman Award

Yaman Arkun, Associate Professor of Chemical Engineering at Georgia Institute of Technology, is the 1986 recipient of the American Automatic Control Council (AACC) Eckman Award for "an outstanding young engineer, under age 35, in the field of automatic control." The award was established in recognition of Donald P. Eckman, who was a professor at Case Western Reserve before he died in a car accident. The American Automatic Control Council–whose member societies are the AIChE, AIAA, ASME, IEEE, ISA, and SCS–is the U.S. National Member Organization of the International Federation of Automatic Control.

Professor Arkun is a native of Instanbul, Turkey. He received his B.S.ChE. from the University of Bosphorous, Turkey, in 1974; and the M.S.ChE. and Ph.D. degrees from the University of Minnesota in 1976 and 1979, respectively. From 1979 to 1985 he was on the faculty at Rensselear Polytechnic Institute. Dr. Arkun is a member of AIChE, IEEE, an Associate Editor of Automatica, and the Vice Chairman of the Systems and Control Area of AIChE.

Dr. Arkun's research interests are in the areas of process dynamics and control, process synthesis, and computer-aided design. Current research topics in process dynamics and control include: modeling needs for process control; synthesis of robust

control systems for complete chemical plants in the presence of modeling errors; development of computer-aided multivariable control system analysis and design software; nonlinear, predictive and robust adaptive control; real-time computer control; and applications of newly developed methods to distillation columns, large scale integrated chemical plants, batch processes, and reactor systems.

In the areas of process synthesis and computer-aided design, some recent studies include the development of dynamic operability measures and the computational tools for large-scale systems; design of chemical plants in the presence of uncertainty; and design of chemical plants with multiregime capabilities.

A recent publication–coauthored with B. Mănouioutghakis, A. Palazoglu, V. Guruswamy, and P. Putz–*"Computer-Aided Analysis and Design of Robust Multi-variable Control Systems for Chemical Processes,"* appeared in Computers and Chemical Engineering **9** (1), 27-59 (1985).
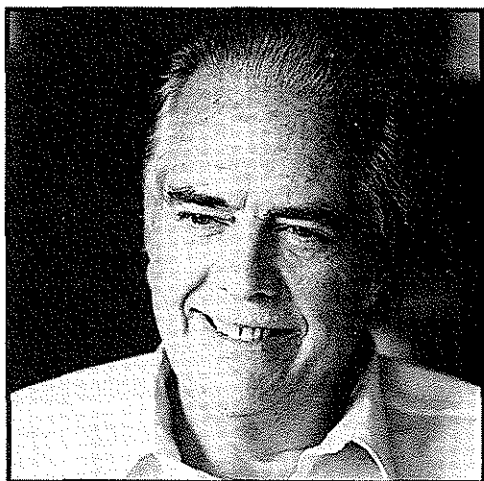
Chemical Engineering Computer Awards

W. McMaster Clarke

Ross E. Swaney Receives the CAST 1986 Ted Peterson Student Paper Award

The Ted Peterson Student Paper Award is given to recognize an outstanding published work, performed by a student, in the application of computing and systems technology to chemical engineering. This award, supported by ChemShare and IBM, consists of $500 and a plaque. The award will be presented on Tuesday, November 4, 1986 at the CAST Division Award Dinner, Fleur de Lis Room, Lobby Level, Chateau Building, Fontainbleau Hilton.

The 1986 winner is Dr. Ross E. Swaney, who is now Assistant Professor at the University of Wisconsin. Ross received his B.S.ChE at Carnegie-Mellon University (CMU) in 1976; his M.S.ChE at CMU in 1978 under Professor Gary J. Powers; his M.B.A in 1980 at the University of Chicago; and his Ph.D. at CMU. His Ph.D. thesis advisor was Professor Ignacio E. Grossman.

Ross was a National Science Foundation Graduate Fellow in 1980-1982, an Exxon Industrial Fellow in 1982-1983, and recieved both the Mark Karl Outstanding Teaching Assistant Award in 1981 and the Graduate Symposium Award in 1982. He was a Senior Engineer at ARCO Petroleum Products Co. during 1977-1980 and 1984. He is a member of AIChE and Sigma Xi.

Dr. Swaney was cited for his paper, *"An Index of Operational Flexibility in Chemical Process Design. Part I,"* AIChE J., **31**, 621 (1985), which was coauthored with his research advisor.

The award nomination statement reads as follows:

"An important problem that arises in the operability of chemical plants is the one of how to analyze the flexibility that a process has for handling uncertainties in parameters such as feed compositions, product demand, ambient conditions, and thermodynamic, kinetic, and transport data.

"Ross Swaney has developed in the cited paper an index of operational flexibility that allows the quantitative assessment of this property. This index provides a measure of the size of the feasible region of operation, which accounts for the fact that control variables in a process can be adjusted during plant operation. This is a crucial point because it gives a realistic measure of the inherent flexibility of a process. Furthermore, this index provides information on the actual lower and upper bounds of the parameters that the design can tolerate, as well as the location of the critical or "worst" point of operation. Also sensitivity analysis information can be easily obtained to determine the required design changes that have the greatest potential of increasing flexibility in design.

"The main contributions of Ross Swaney have been to develop rigorous mathematical formulations for this index, and the development of effective computational schemes to solve the difficult max-min-max problems that arise in the formulations. Here an important accomplishment was to determine the flexibility index without having to solve the 2 to the nth power nonlinear programs for each parameter vertex. The examples that were solved in the paper clearly show that the proposed procedures can be used effectively to quantify flexibility in chemical processes.

David M. Himmelblau is the Recipient of the 1986 CAST Computing in Chemical Engineering Award

The Computing in Chemical Engineering Award is given in recognition of an outstanding contribution in the application of computing and systems technology to chemical engineering. The award, supported by Intergraph and Simulation Sciences Inc., consists of $1500 and a plaque.

The 1986 winner is Professor David M. Himmeblau, the Bob R. Dorsey Professor of Chemical Engineering at the University of Texas, Austin. David will receive the award and will speak on, "A Personal Perspective on Computing," at the CAST Division Award Dinner on Tuesday, November 4, 1986 Fleur de Lis Room, Lobby Level, Chateau Building, Fontainbleau Hilton.

The award citation reads as follows:

"David M. Himmelblau is a model of the complete university professor of chemical engineering. He is an extremely able lecturer and faculty advisor. He has diversified interests in the many facets of professional education, including not only his university courses but also continuing education courses, the preparation of modular instructional materials as executive director of an organization (CACHE) devoted to aiding chemical engineering educators, and as a consultant. He has maintained a contemporary research program in process analysis, optimization, and computer-aided design."

David received his B.S.ChE in 1947 at MIT, his M.B.A. in business administration in 1950 at Northwestern University, and his Ph.D. in chemical engineering in 1957 at the University of Washington. David's technical and professional society memberships and offices include Vice Chairman of the CAST Division, 1980-1981; Chairman, CAST Division, 1981-1982; Director, AIChE, 1974-1976; Chairman of three national committees since 1962; ASEE Executive Committee, ChE Division, 1970-1971; ACS, Chairman, Central Texas Section, 1967-1968; and member of the editorial board of I and EC Process Design, 1972-1975. He edited the "ChE Faculties" and Student Member Bulletin for several years. He has been an active member and Vice President, President, and Executive Officer of CACHE, of which he has been a Trustee for 12 years. He received the CACHE Award for Contributions to Chemical Engineering in 1980 and was elected Fellow of the AIChE in 1980. David is a member of AIChE, the American Mathematical Society, SIAM, and ASEE. He is listed in Who's Who in America, American Men of Science, Who's Who in Engineering, and similar publications.

According to a supporter of the the nomination: *"Perhaps the most significant professional activity that Dave has undertaken is the writing of key textbooks in a variety of fields: (1)* **Basic Principles and Calcuations in Chemical Engineering**, *a book (first edition in 1962) that has had amazing longevity for a chemical engineering textbook; (2)* **Process Analysis and Simulation** *(1968, co-authored by Ken B. Bischoff), one of the first books on mathematical modeling for chemical engineers; (3)* **Process Analysis by Statistical Methods** *(1970), still a valuable reference book that is a broad compendium of useful information; (4)* **Applied Nonlinear Programming** *(1972), perhaps the first book written for engineering*

researchers in the field of optimization (a successor to Beveridge and Schechter); (5) **Fault Detection and Diagnosis in Chemical and Petrochemical Processes** *(1979), which now stands as a key reference in the field of artificial intelligence for chemical enginering processes; and (6)* **Optimization of Chemical Processes** *(1986, co-authored by Thomas F. Edgar)."*

His contributions to the literature were summarized as follows:

"He was among the first chemical engineers to develop optimization tools for chemical engineering design problems. His work with Paviani in 1969 led to the development of one of the first successful software packages for large scale process optimization. This work has continued over 15 years. He has led in the development and use of decomposition methods for solving equation-based flowsheets, as exemplified by his publications with Ledet in 1970 and his book in 1973. He has pioneered the use of large mainframe computers to examine the stochastic aspects of the design of unit operations, and has essentially opened this important field of research for the chemical engineering community. This has been documented in his publications with Beryman (1973), Kado (1973), Cockerham (1974), Mistry (1975), Tanthapanichakoon (1980), and Park (1980). He has done innovative research on waste water treatment, solar energy modeling, and coal gasification modeling. Finally, he has recently contributed to seminal work in fault detection with Park (1982) and Watanabe (1982, 1983). All of the above reveal a very active researcher working in a number of fields that are unified by their dependence on large scale digital computation and the application of creative ideas to difficult problems."

Please use the form on the two pages at the end of this issue to submit your nomination for the 1987 Computing in Chemical Engineering Award and the 1987 Ted Peterson Award. Eight copies of the nomination for the Computing in Chemical Engineering Award, and four copies of the nomination for the Ted Peterson Award, should be sent by April 2, 1987 to W. M. Clarke, Olin Chemicals, P. O. Box 248, Lower River Road, Charleston, TN 37310.

Chemical Network Problems Solved on NASA/Goddard's Massively Parallel Processor Computer

Gregory R. Carmichael, Seog Y. Cho, and David M. Cohen*, Department of Chemical and Materials Engineering and *Department of Computer Science, University of Iowa, Iowa City, IA 52242

Abstract

The single instruction stream, multiple data stream MPP processor consists of 16,384 bit serial arithmetic processors configured as a 128 x 128 array whose speed can exceed that of current supercomputers (Cyber 205). This paper presents and discusses the applicability of the MPP for solving reaction network problems, as well as the machine architecture, the mapping of the calculation to the architecture, and CPU time comparisons.

I. Introduction

A detailed model which describes the transport and removal of photochemical oxidants, and acidic species and precursors in the troposphere has been under development for the past nine years. The present analysis consists of about 30 coupled three-dimensional time-dependent nonlinear partial differential equations and about 50-100 coupled nonlinear ordinary differential equations.

The model is representative of a number of comprehensive Eulerian transport/chemistry models being developed for regional air pollution problems. However, these models are only feasible when run on "supercomputers." Our model was developed originally on the NASA-Langley CDC-STAR computer and is currently on the NASA-Langley Cyber 205, the NCAR CRAY-1 and a FAC M240 at Nagoya University, Japan. The execution times are 0.025 CPU-sec/grids-time step on the FAC M240, 0.007 CPU-sec/grids-time step on the CRAY-1, and 0.70 CPU-sec/grids-time step on a VAX 11/780. Thus, a 24-hour simulation on the CRAY-1 for the eastern United States with 9500 grid points requires 100 CPU-minutes. Typical applications require simulations of seven to ten days.

Our experience has shown that transport/chemistry models can execute about 70-100 times faster on the "supercomputers". However, 100 CPU-minutes/simulation-day is still too large for most applications. Therefore, to exercise these models, various simplifying assumptions are used to decrease the CPU time. However, these assumptions add additional errors and uncertainties to the model results. Faster computers will enable the execution of the "best-science" model version.

Currently about 90% of the CPU time is spent doing the chemistry calculations. The chemistry introduces the stiffness, the coupling and the nonlinearity into the model. Thus, the highest priority in continued model development is to search for ways in software and hardware to reduce the chemistry calculations. The purpose of this paper is to describe our attempts to exploit a massively parallel computer architecture to accelerate the chemistry calculations.

The MPP is a unique, single instruction stream, multiple data stream processor. It consists of 16,384 bit serial arithmetic processors configured as a 128 x 128 two-dimensional array and is controlled and accessed through a VAX 11/780 computer. Initial trials indicate that the MPP processor speed can exceed that of current supercomputers. For example, a shallow water model executes three to four times faster on the MPP than on a Cyber 205. This paper will report on the applicability of the MPP for solving reaction network problems. The machine architecture, the mapping of the calculation on the architecture, and CPU timing comparisons are presented and discussed.

II. Model Overview

The regional-scale combined transport/chemistry/deposition model is Eulerian and treats 50 chemical species. Thirty species are advected, while the remaining species are short-lived and are modeled using pseudo-steady-state models. The mathematical analysis consists of partial differential equations for the transported species and additional algebraic equations for the steady-state species. The transported species satisfy

$$\frac{\partial C_i}{\partial t} + \nabla \left(V C_i \right) = \nabla \bullet K \bullet \nabla C_i +$$

$$R_i + S_i - G_i, i = 1, \ldots , 30; \quad (1)$$

where C_i is the gas-phase concentration of the ith chemical species, V is the wind velocity vector, K is the eddy diffusivity tensor, R_i denotes the chemical reaction term, S_i is the source term, and G_i is used to describe the mass transfer between the gas and condensed phases. The algebraic equations for the gas-phase species assumed to be at steady state are written as

$$R_i \left(C_1, C_2, \ldots , C_{50} \right) = 0,$$

$$i = 31, \ldots , 50. \quad (2)$$

These equations are representations of general chemically reactive flow problems.

Simulation of regional transport, chemistry and deposition as described by Equations (1) and (2) requires numerical integration. The method presently used is a combination of the concept of fractional time steps and one-dimensional finite elements. This is referred to as Locally One-Dimensional Finite-Element Method (LOD-FEM). The LOD procedures (Mitchell, 1969) split the multidimensional partial differential equation into time-dependent, one-dimensional problems which are solved sequentially. The transport equations are solved using a Crank-Nicolson Galerkin finite element technique. Chemistry and mass transfer equations are solved using an adaptation of the semi-implicit Euler method proposed by Preussner and Brand (1981).

III. Overview of the Massively Parallel Processor

A. Hardware

The Massively Parallel Processor (MPP) was built by Goodyear Aerospace for the NASA Goddard Space Flight Center. It operates as a peripheral processor to a host machine (DEC VAX 11/780).

The four major components of the MPP are shown in Figure 1. The Array Unit (ARU) consists of a 128 x 128 array of Processing Elements (PEs), either open at the edges or connected to form a horizontal cylinder, a vertical cylinder or a torus. Each PE contains a full adder, a variable length shift register (2-30 bits), logic circuitry, 1024 bits of random access memory, and various registers (see Figure 2).

Instructions for the ARU are issued from the Array Control Unit (ACU). As shown in Figure 3, the ACU has three distinct parts, any number of which may execute simultaneously: the Processing Element Control Unit (PECU), the I/O Control Unit (IOCU), and the Main Control Unit (MCU). The PECU and the IOCU send instructions to the ARU, while the MCU serves as a fast serial processor which invokes the PECU and IOCU functions as subroutines. All array manipulations are performed by means of the PECU; all scalar arithmetic is programmed in the MCU. The IOCU manages the flow of data into the ARU.

The Program and Data Management Unit (PDMU) of the MPP consists primarily of the DEC PDP-11/34 minicomputer. It manages data flow into the ACU, performs diagnostic tests of the hardware, and buffers output to secondary storage devices, terminals and printers.

The Staging Memory Unit (SMU) consisting of 32 Mbytes of storage lies in the data path between the host computer and the ARU-PDMU components of the MPP. Its function is to buffer and/or reformat arrays of data.

The ARU has an instruction cycle time of 100 nsec. Peak performance of the MPP with respect to manipulation of 128 x 128 arrays has been reported in the literature (Hwang et al, 1984). Using 12-bit integers, array addition can be performed at 4428 mops (millions of operations per second), element-by-element multiplication of two arrays (Hadamard product) at 910 mops, and multiplication of an array by a scalar at 1260 mops. Using 32-bit floating point numbers, the peak performance rates are 430, 216, and 373 mops, respectively.

B. Programming Considerations

The MPP belongs to the class of SIMD (single instruction stream, multiple data stream) computers. Unless disabled for a particular machine cycle, each PE performs the same operation as all the other PEs. Addition and multiplication of arbitrary length integers and floating point numbers is accomplished through successive operations on the individual bits of the operands.

A bitplane is an assignment of bit values to each PE. Each bitplane represents one bit of each of 16,384 numbers. A 32-bit integer, for example, would be represented as 32 bits in the local store of the single PE. A collection of 32 bitplanes would characterize a "parallel array" of 32-bit integers.

The assembly language for the Processing Element Control Unit is called PEARL (PE Array Language). All operations on bitplanes or on parallel arrays are accomplished by the use of PEARL subroutines. Microprogram

conflicts are detected by the PEARL assembler.

The programming language for the I/O Control Unit and the Main Control Unit is MCL (Main Control Language). Macro processing is available, as well as the ability to define parallel array variables corresponding to collections of bitplanes in the ARU. Parallel array variables may be of several types, including (arbitrary length) integer, 32-bit floating point, and bitplane.

C. Programming Environment

The MPP is designed to run in tandem with the VAX 11/780. The Parallel Pascal Compiler accepts a language which is an extension to Pascal (allowing for parallel array variables among other things) and produces code for both the MPP and the VAX (see Figure 4).

A symbolic debugger is available to help the user correct errors in MPP programs. CAD (Control and Debug) is an interactive tool, allowing for the display and modification of values in the MPP registers and for the alteration of the control flow of the program.

VAX-resident code is assembled and linked with host libraries, user-suppled subroutines and the MCU symbol table. MPP-resident code is assembled and linked with MCU libraries and routines and PECU routines ("primitives"). The VMS load module, PECU load module, and MCU load module are the outcome of the compilation and link steps.
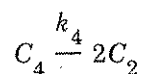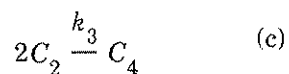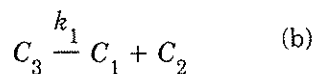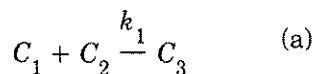
With regard to program organization, one may choose to let the Pascal main program reside in either the VAX or the MPP. Alternatively, the MPP-resident code could be called as subroutines from VAX-resident programs written in other languages (e.g., in FORTRAN).

D. Comparison with Other Machines

The performance of the MPP may be compared to that of two other SIMD computers (Gabriel, 1986; Lerner, 1985). The Connection Machine (Thinking Machines, Inc.) has 65,536 1-bit processors connected in the Boolean n-cube. Each processor has 4096 bits of local memory and 16 registers. The Non Von computer (Columbia University) has 64 processors (to be increased to 8000 in the near future) which may operate in either an SIMD mode or an MIMD (multiple instruction stream, multiple data stream) mode. There are two categories of processors, small PEs (8-bits) and large PEs (32-bits). The small PEs are connected as a complete binary tree, with the leaf nodes connected to each other in a two dimensional grid. Subsets of small PEs act in unison as a SIMD machine, under the control of a large PE. The MPP, the Connection Machine and Non Von have maximum speeds of 6.5, 10, and 16 BIPS (billions of instructions per second), respectively.

IV. Test Problem: Chemical Network Problem

To evaluate the ability of the MPP to calculate chemical network applications a simple four species test problem was selected. The four species (C_1, C_2, C_3, C_4) are involved in the following chemical reactions:

$$C_1 + C_2 \overset{k_1}{-} C_3 \qquad (a)$$

$$C_3 \overset{k_1}{-} C_1 + C_2 \qquad (b)$$

$$2C_2 \overset{k_3}{-} C_4 \qquad (c)$$

$$C_4 \overset{k_4}{-} 2C_2$$

The transport equations describing this system is represented by Equation (1) with i = 1, 2, 3, and 4.

As mentioned in the model overview section, one way of numerically solving complex transport chemistry network problems is to split the equation into transport and chemistry parts. The chemistry calculations using this technique requires solving the set of equations

$$\frac{\partial C_i}{\partial t} = R_i \quad i = 1, \ldots, \# \ of \ species \quad (5)$$

at each grid point in the discretized space.

The use of the semi-implicit Euler method to solve Equation (5) results in the equations

$$\frac{dC_i}{dt_r} = -C_i + \sum_j d_i^j \prod_{k=1} C_k$$

$$+ \sum_\ell P_i^\ell \prod_m C_m = 1, \ldots, 4 \quad (6)$$

This set of ODE-IVP's is solved within each transport time step, i.e., $t_o \leq t_r \leq t_{transport}$.

Now consider the case when we have 16,384 grid points in discretized spatial domain. Therefore each chemical calculation within each transport step requires the solution of 16,384 sets of Equation (6). To implement the solution of these equations on the MPP requires first the choice of how to map the equations to the architecture. In this case we have chosen to simply view each processor as a grid point in the discretized space, and to have each processor solve its own set of Equation (6). The algorithm for solution of Equation (6) is written in Parallel Pascal and resides on the VAX.
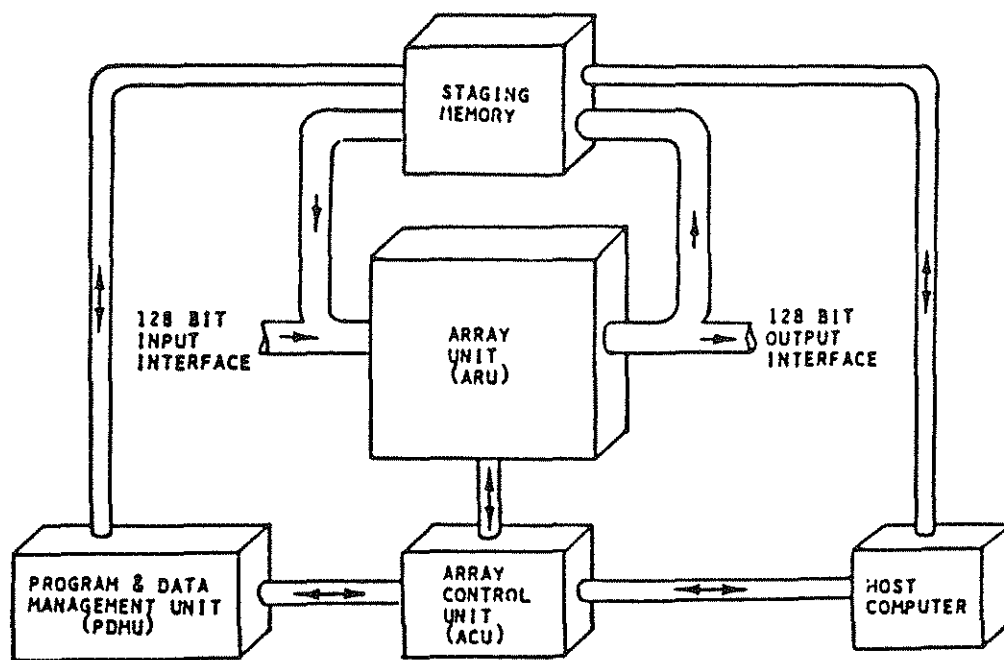
Figure 1. MPP System Block Diagram
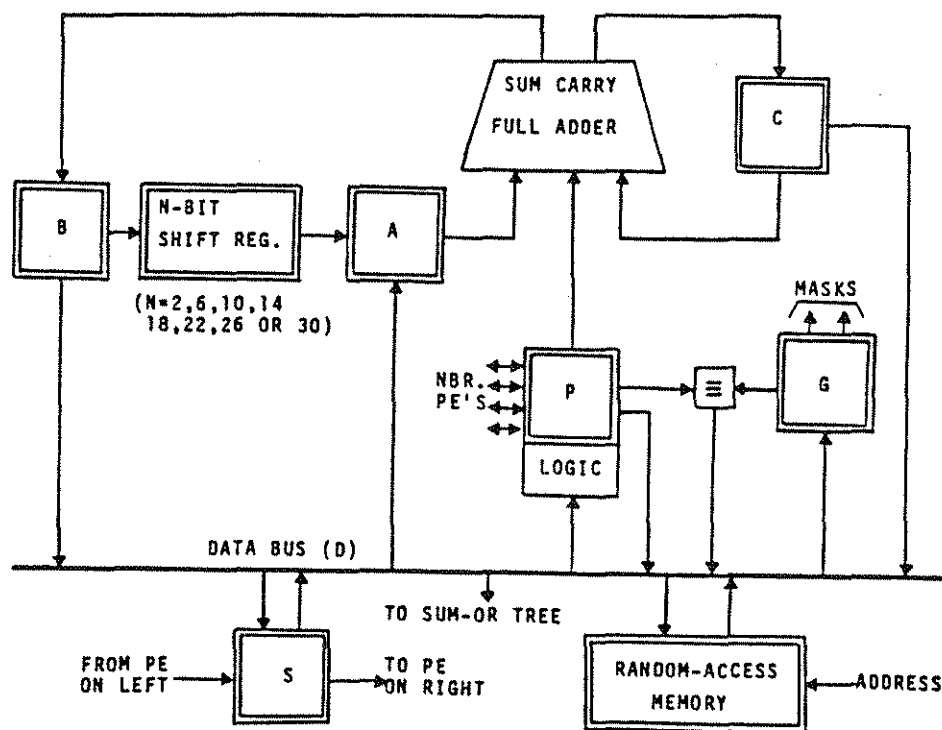
Figure 2. Functional Units of One PE

PECU   IOCU   MCU

PE CONTROL UNIT	I/O CONTROL UNIT	MAIN CONTROL UNIT

LANGUAGE:
PEARL   MCL   MCL

Figure 3. The Array Control Unit (ACU)

PARALLEL PASCAL

```
        SOURCE CODE
             |
          COMPILER
             |
           P-CODE
             |
       CODE GENERATOR
          /        \
VAX MACRO SOURCE    MCL SOURCE    MACRO LIBRARY
       |              |
VMS MACRO ASSEMBLER  MCL ASSEMBLER
       |              |
VAX OBJECT MODULE   MCU OBJECT MODULE
       |              |          PRIMITIVE LIBRARY
       |            MPP LINKER
VAX RUNTIME         /      \     MCU RUNTIME LIBRARY
LIBRARY      MCU SYMBOL TABLE
       \      /
     VMS LINKER
         |              |
  VMS LOAD MODULE   MCU LOAD MODULE
```

Figure 4.   MPP Pascal Program Development Steps

The CPU time required for execution of 100 time steps on the MPP of this 4 species mechanism at 16,384 grid points is 0.293 CPU-seconds. The same problem was executed on the VAX-11/780 and required 138 CPU-seconds. Thus for this chemical network problem the MPP executed a factor of 470 times faster than VAX 11/780!!

The above test calculation indicates the MPP is well suited for chemical network problems where each node can hold the entire mechanism. Current memory restrictions limit the size of the chemical mechanism that can be solved in this fashion. At present each processor can hold 32 32-bit variables. (It is planned to increase the storage in the near future.) However, it is possible to handle larger chemical mechanisms. One way is to group processors together. For example, if 128 words are required at each node then four processors can work together. This in turn would reduce the maximum number of grids possible by a factor of 4. Another way is to make use of the staging memory.

We are in the process of implementing the total transport and chemistry calculation on the MPP. The plan is to perform the chemistry calculations on the MPP-side and simultaneously perform the transport calculation on the VAX-side; thus exploiting both the massive parallelism on the MPP and the concurrency between the VAX and the MPP.

Summary

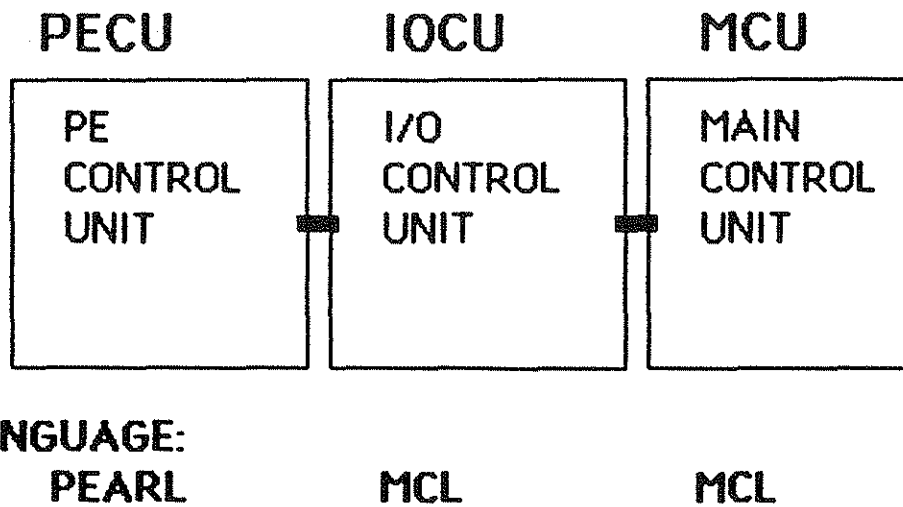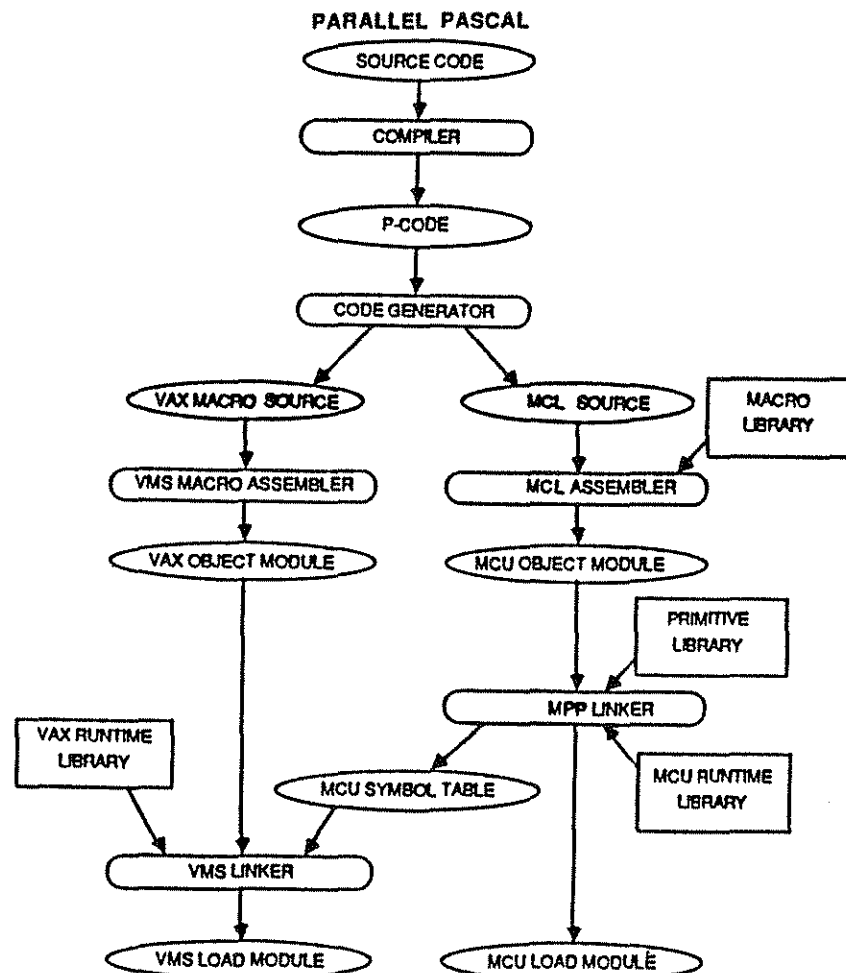The suitability of the MPP computer for calculation of network problems is under evaluation. To date the MPP has been used to calculate a test problem which represents one component of a complicated chemically reactive flow problem. Specifically the set of coupled ODE-IVP's describing the chemical reactions occurring at 16,384 spatial grid points was calculated.

This problem is ideally suited for the MPP because by using operator splitting, the chemistry at each grid point acts independently from that of the other grids (within each transport time step). This test calculation showed that the MPP can perform the calculation 470 times faster than the VAX 11/780. Also since nearly 90% of CPU time of large chemically-reactive flow problems is spent doing the chemistry calculations, the MPP architecture offers great potential for CPU savings for model applications.

Acknowledgments

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Doe Workshop on Research needs in Energy Engineering: Systems, Instrumentation, and Control

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I.   Introduction

The processes and machinery involved in energy production, transmission, conversion, conservation, and use rely increasingly on automated operations and control. Automation of such processes can reduce labor requirements, achieve greater productivity and reliability, increase efficiency, reduce waste, and maximize quality and repeatability. Thus automated systems are normally preferred over manual operations, especially in hostile environments. Development of automated facilities involves an understanding of the mechanics and behavior of their processes (systems analysis or engineering modeling) and requires sensors, transducers, communications, and actuators to carry out the automated activities ("instrumentation"). However, the key to the success of an automatic system is a "brain" that determines how measurements are converted to actual commands. This part of the total package is the control "intelligence," often taking the form of control algorithms implemented in a computer software program. Systems, instrumentation and control are

integral components of an automated process.

II. Application

The applications of new systems control and instrumentation technology of relevance to energy can be broadly categorized into four main areas: (1) fuel exploration, (2) fuel production, (3) energy production and utilization, and (4) waste product utilization and disposal. These areas are discussed below.

A. Fuel Exploration

Great advances have occurred during the last thirty years in technology for exploration of fossil and nuclear fuels using advances in sensors and analysis of the resulting information. These include remote sensing techniques and down-hole logging methods for resource location and for characterization of the resource and geological medium. Most of this technology has been developed within the private sector, and this situation is expected to continue. However, the potential use of intelligent, autonomous machines in fuel exploration will require basic research, which is in the purview of DOE.

B. Fuel Exploration

Systems control and instrumentation has been applied to oil and gas recovery (including secondary and tertiary production), production of fuels from oil shale, coal, and tar sands, either by *in situ* or conventional methods, and uranium production. Much of the planning, scheduling and optimization in fuel production must be based on simulators, many of which are large-scale in nature, even requiring a supercomputer for satisfactory operation.

C. Energy Production and Utilization

This multifaceted area involves energy in many forms and uses, and includes primary technologies such as coal-fired and nuclear-based generators. However, there is great potential for new applications in energy utilization and delivery, including such areas as transportation, processing, manufacturing, and power systems. Each area has specific characteristics that influence the nature of the basic research that should be undertaken.

The worldwide transportation system is truly gigantic, and thoroughly interconnected and interactive. The parallel highway, rail, waterway, and airway systems are all subject to concerns such as efficiency, reliability, energy consumption, and scheduling.

An oil refinery is typical of process plants that involve the coordination of thousands of pieces of equipment and flow scheduling of a variety of raw materials and products under the control of a large computer system at the heart of a measurement and communications system.

Manufacturing refers to discontinuous operations, such as single product lines in an automobile assembly line. In addition to transportation, warehousing, and scheduling considerations, coordination of machines to manufacture products with different parts and characteristics in a random sequence often creates an even more complex scheduling problem than with continuous processes.

Energy delivery involves gas and oil pipelines, tankers, and large electric power systems. The latter is one of the largest of systems, involving almost 10,000 large generators with the time scale of phenomena ranging from microseconds (for lightning-induced transients) to years (for construction of

power plants). Some aspects of its operation include load frequency control and optimal load storage and dispatch, load management and peak load reduction, security analysis to ward off emergencies, system stability analysis, automated equipment maintenance, coordinated control of the generating units, and interactions with environmental and other governmental regulations.

D. Waste Product Utilization and Disposal

An important consequence of energy systems is the waste that results from the production, conversion, or utilization of fuels. These include waste heat, gaseous and liquid pollutants, and solid waste, and their impact on air and water quality. Waste products arising from nuclear operations and toxic chemicals have received great visibility recently, especially because of the threat to groundwater supplies. Disposing of such wastes involves rather complex interactions between societal and legal regulatory concerns. A systems approach must be used to balance environmental damage and safety concerns against the energy needs of the population.

III. Research Needs

High priority research needs in the areas of systems, instrumentation, and control are given in this section. Twelve research areas (see Table 1) have been selected as the most significvant ones for inclusion in the U.S. Department of Energy Engineering Research Program. These topics were selected based on satisfying all of the following criteria:

(1) The research would enhance energy efficiency and would minimize associated risks in its production and utilization;

(2) The problem solution will potentially have a large impact on energy technologies into the 21st century;

(3) The research results will fill gaps in existing knowledge for control, or open new fields of controls in energy technology;

(4) The research will contribute to fundamental knowledge for control and measurement in the energy field.

We summarize each of the four major classifications in Table 1 below.

In addition to the twelve areas mentioned in Table 1, a number of other research areas were considered to be important, but at a lower (but still important) priority. These are shown in Table 2 using the categories in Table 1.

A.   Research Needs in Sensors

Sensors are a vital link in modeling and control of physical systems. Information from sensors can be used to validate mathematical models, to analyze process behavior, to determine difficult-to-measure properties or parameters, to improve or optimize processes and to improve operability. Sensors are also used in the context of control, where they provide a measurement of the quality of the process output. Feedback control cannot be implemented without accurate information on the process variables, which is provided by sensors. When the primary output variable is not measurement in real time (i.e., too slow to influence the process in a dynamic state), then secondary measurements must be analyzed to infer the values of the desired output variable. While the cost of control computers has declined in recent years, sensor costs continue to be a major component in the overall system cost. Further, the very nature of modern control mathematics

dictates a higher level of measurement accuracy than that for older analog systems, which also leads to higher costs for the sensors. Therefore, it is desirable to develop inexpensive, reliable, and accurate devices for measurements for a wide variety of energy applications. Such devices may be passive (requiring only a detector to pick up a signal already in the process) or active (requiring a transmitter-detector pair to sense changes in the transmitted signal).

Table 3 details the typical uses of sensors in each phase of the energy cycle discussed in section II. The four high priority research areas given in Table 1 are generic in nature, in that they apply to a range of application areas. For example, multiphase flow measurement is required in both fuel and energy production, and in utilization. Examples are solid-liquid slurry flows in a coal conversion plant and gas-liquid flow in boreholes. What is needed are reliable devices for the measurement of two- or three-phase flow for both above-ground and subsurface applications. These devices should function reliably over a wide range of flow rates and phase ratios as well as at pressures up to 25,000 psi and temperatures up to 1000 C (however, all capabilities will not be provided by a single device).

In situ analysis of chemical composition and physical properties has importance in coal conversion, fossil fuel exploration and production, and chemical processes in general. The monitoring of chemical composition is very important in combustion processes, where it is necessary to know the composition of the fuel components as well as the nature and amounts of potential pollutants, which may exist only in trace quantities. New spectroscopic methods are particularly attractive. Research is also needed on methods to characterize the physical properties of

geological media located far from the sensor.

Conventional instruments, when used in harsh environments such as high temperatures and pressures, often do not exhibit satisfactory endurance or reliability. Nor are such instruments self-calibrating or self-checking ("smart"). Energy recovery processes often operate at high temperatures; combustion is a typical example. High pressures are found in coal conversion plants making synthetic natural gas or oil. In hostile environments, human calibration is not always feasible.

The integration of information from multiple sensors is another high priority research need. Such integration implies a model of the process being monitored, a rational for rejecting spurious measurements, handling noisy measurements, combining measurements of varying quality, and the use of such measurements in process control. Software needs to be developed which reduces existing filtering theory to practice. Applications of this technology are in robotics and in chemical processes.

B.   Research Needs in Control Systems

Implementation of control intelligence is a key part of a functioning process control system, since without a sufficient level of intelligence the system might fail to meet performance specifications or even become inoperable due to instability. The design of control algorithms is well established for processes of modest scale (i.e., linear processes with a single measurement, a single control point, and fewer than 20 state variables). As the scale, complexity, and dimensionality of energy processes grow, existing control theory faces more demanding design problems, leading to the need for new design

Table 1.   High Priority Research Needs–Systems, Instrumentation, and Control

A.   Sensors

    1.   Multiphase flow measurement
    2   *In situ* analysis of chemical composition and physical properties (including combustion)
    3.   Smart sensors for high reliability in harsh environments
    4.   Integration of information from multiple sensors

B.   Control Systems

    1.   Nonlinear control
    2.   Multivariable control
    3.   Robust control of uncertain systems
    4.   Adaptive and self-learning control

C.   Modeling, Simuation, Software, and Languages

    1.   Concurrent computation for control and for sensor integration
    2.   General purpose control system simulation and control system design of software/languages

D.   Large-Scale Systems

    1.   New techniques for modeling and control
    2.   Systems diagnosis and reconfiguration under fault/failure conditions

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Table 2.   Research Topics of Secondary Priority–Systems, Instrumentation, and Control

A.   Sensors

    1.   Measurement of physical properties of the earth
    2.   Optical sensors and fiber optic techniques
    3.   Time-varying imagery

B.   Control Systems

    1.   Real-time optimization
    2.   Control and measurement of configured designs
    3.   Control of distributed parameter systems
    4.   Smart actuators for control
    5.   Interrelationships of modeling and control
    6.   Control of multi-degree-of-freedom systems
    7.   Computational structures and architectures for control

C.   Modeling, Simulation, Software, and Languages

    1.   Models for complex energy-related systems
    2.   Object-oriented software for control design and system diagnosis
    3.   Symbolic manipulation software and control

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principles and tools to solve these problems.

Most energy processes exhibit strong nonlinear behavior in their static as well as dynamic characteristics. Until recently, control theory has offered few tools to deal with such processes. Established practice calls for linearization of the process model, followed by control design with classical linear methods and by *post-hoc* design adjustments to account for known nonlinearities. The design adjustments are normally based on

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Table 3.   Sensor System Application Areas

Phase of the Energy Cycle	Sensor System Application
1. Fuel Exploration	
● Oil and gas exploration ● Uranium exploration	● Resource location ● Resource characterization ● Characterization of geologic medium
2. Fuel Production	
● Conventional oil and gas ● Unconventional fuel production (oil shale, underground coal gasification, tar sand) ● Uranium production	● Characterization of geologic medium ● Estimation of resource size ● Measurement of recovery rate ● Monitoring of recovery process ● Measurement of environmental impacts of recovery
3. Energy Production and Utililization	
● Conventional gas or coal fired ● Production from unconventional fuels ● Nuclear ● Hydroelectric	● Validation of process model ● Metering of constituents for power generation ● Control of energy generation process ● Monitoring and control of effluents ● Verification of safe operating conditions ● Emergency shutdown
4. Waste Product Utilization and Disposal	
● Waste heat ● Waste liquids ● Solid wastes ● Nuclear wastes	● Monitor and control waste product utilization ● Monitor disposal rates ● Monitor effect of disposal on biosphere ● Verify safety of disposal process

extensive simulation evaluations. Recent theoretical work in nonlinear dynamical systems shows some promise. One approach attempts to contain the nonlinearities within linear boundaries. Other nonlinear systems which are not too large can be treated by using nonlinear feedback control to linearize the closed-loop properties. Once this property is obtained, much of the theory used for linear systems can be extended to nonlinear ones. The research area of nonlinear system control is relatively immature and thus deserves additional effort.

While most energy processes are nonlinear, many can still be treated successfully with linearized models. Unfortunately, even linear models often challenge the design capabilities of available control theory. This happens when processes have many measurements and many control points instead of just one of each, and also when the automatic system must operate successfully despite large modeling errors (large differences between the actual controlled process and the model used for design). Two interrelated subsets of control theory that attempt to deal with these latter design situations · are called

"multivariable control" and "robust control," respectively. Both areas have experienced substantial progress in the last few years. Some highlights include the introduction of "singular values" as correct multi-variable generalizations of the classical single-input, single-output Bode gain functions; the use of singular values as measures of stability robustness of multivariable feedback loops (i.e., how much modeling error can be tolerated before instability occurs); and their use in classical frequency domain interpretations of the modern Linear-Quadratic-Guassian (LQG) design methodology. Future research should

aim to develop control algorithms with prescribed performance and robustness properties for the large multivariable processes common to the energy industries.

Control theorists have long striven to develop "smarter" control algorithms with the capacity to adjust themselves to process characteristics, and thus to be inherently insensitive to modeling error as well as to be more finely tuned to performance characteristics. Such algorithms are called "adaptive" or "self-learning" by controls specialists and are an alternative to robust controls with pre-designed tolerance for large modeling errors. Today, they might well be called "artificially intelligent."

Adaptive control theory has thus progressed from heuristic enginering adaptation to more formal mathematical studies. Control algorithms based on recent theoretical advances can be made to work for specific problems, but they do not work consistently well. Heuristic control schemes have proved unstable in some applications (or at least require occasional resets). Formal mathematical schemes, while globally stable under the stated assumptions, can become unstable when those assumptions are violated even in seemingly innocent ways. However, new theories for robust adaptive control can be developed, and should yield algorithms that are consistent and reliable over a wide range of energy applications.

C. Modeling, Simulation, Software, and Languages

There are several technological developments that will stimulate new software generation. Data acquisition will increase as computers become more ubiquitous, so it is important to decentralize the use of such data, perhaps by using new hardware such as Very Large Scale Integrated (VLSI)

circuits. Self-checking and self-calibrating sensors and activators will be developed, along with controllers that have enhanced capabilities (such as symbolic manipulation) and more advanced man-machine interfaces. With this new hardware, there will be a need to develop new software (perhaps not based on FORTRAN). The new software should facilitate communication between the operator and the computer (perhaps using so-called natural languages), should aid in on-line knowledge-building, and should provide consistency and reliability checks. Specialized languages for simulation and control will also be neded, both for off-line and on-line computations. Computer networks will become crucial to successful management systems and to control systems, both of which will be of the "distributed" type.

Dynamic simulators are slowly supplanting steady-state simulators as designers become more concerned with plant operability, reliability, and flexibility. Steady-state simulators, which are available commercially in a variety of application areas, do not provide adequate guidance for designing control systems. We may expect the economic viability of most manufacturing plants to increase with improvements in facility automation and control. There is a need for a general simulation utility for manufacturing flowsheets (especially for discrete systems), to provide interactive design for facilities characterized by nonlinearities and multiple inputs and outputs. A simulator can be used to plan operations, to perform troubleshooting, and to carry out fault diagnosis. In addition, the simulators can be used in operator training, especially in dealing with abonormal conditions. Such a flowsheet simulator, whether for discrete parts manufacturing or for a chemical plant, should have the following characteristics: (1) good physical

property data bases, (2) robust, proven integration routines, and (3) good diagnostics.

The typical discrete manufacturing or batch plant is a multipurpose plant, where the processing sequence for each product is quite distinct. The prototype plant consists of a collection of process equipment which may be configured directly for each product, perhaps also involving variable operating conditions. There is a known demand for a certain amount of each product. The scheduling problems associated with such an operating system are quite challenging and involve some staggering combinatorial optimization problems. Compared to continuous processes and their simulators, the current state-of-the-art for simulating and solving such problems is far from satisfactory.

There is a need for fundamental research on identifying the important structural properties of these systems and methods of decomposition of the structures. Efficient optimization/suboptimization algorithms are necessary to solve the scheduling problems, and some methodology for estimating the benefits of optimal scheduling is needed.

There is also a need for general purpose control system design programs, especially to serve as a medium of transfer of new control technology from universities to industry. The emphasis here is on reliable algorithms embedded in software packages that are user-friendly and easy to debug. There has been considerable development recently in algorithms for multivariable control, adaptive control, robust control, and nonlinear control, but none of these algorithms appear in currently available control systems design software packages.

Recently there has been more emphasis in process control on using modern languages such as LISP, ADA, and C rather than FORTRAN. In the field of software and language development, one area receiving the greatest interest currently is a type of programming referred to as "object-oriented" programming. Much of the importance for object-oriented programming comes from the burgeoning field of artificial intelligence as well as the need for improved man-machine interfaces. The structure of this language is configured like a tree, so that a user can follow various branches in the tree to a code or piece of information that is of interest. The language makes extensive use of icons (e.g., coresponding to pieces of equipment or activities).

Advances in parallel-processing machines should also have some impact on the design of control systems constrained by a heavy computational effort or a very short process response time. An example might be a complicated simulation of combined fluid flow, heat transfer, and mass transfer, such as would occur in coating of various polymeric or metallic films or in crystal growth. In this application, sets of partial differential equations, often of a boundary value nature, must be integrated to determine appropriate control actions. Very little research has been carried out on this topic but it is one that should be very important in the next decade.

D.   Large-Scale Systems

Interconnected networks of very large dimension characterize energy-connected systems such as electric power systems, transportation systems, production and warehousing systems, communications systems, robotic and large manufacturing systems. They consist of many elements, often similar, that interact in an either equal or subordinated way and are influenced by a hierarchy of computers–micro, mini, and macro. Existing control theory can deal with a few subproblems in such systems, but it cannot successfully treat the control of an entire large, coordinated system, or guide the restoration of a failed system. Clearly, there is a need to develop a truly large system theory by the 1990s.

This theory should include the following subject areas:

(1) *Feature determination*–to account for unconventional features in very large systems with hundreds of thousands of interacting dynamic elements.

(2) *Quantitative representation*–to express system conditions where conventional dynamic state concepts do not exist, are unknowable, or are too large to handle.

(3) *Control modeling or control action representation*–to develop control laws which are computable in real time.

(4) *Exploitation of structure for control*–to describe such characteristics as hierarchies, concurrent computation, network interactions, decoupling, decentralization, or models of the non-differential equation type.

There are two extremes in large-scale system structure:

(1) A pure hierarchical structure, where the subsystems are arranged in hierarchical layers, with the interactions forming a pure tree-type graph.

(2) A pure network structure, which consists of subsystems of equal hierarchical rank, each interacting with a limited number of nearby subsystems only.

Large-scale systems can incorporate varying amounts of the two extremes. In large systems, such as those that occur in digital communications or discrete manufacturing, the normal definition of a state variable may not apply. "State" in these cases might mean a multitude of binary positions, the dynamics coming in delays or queues, rather than in the form of differential equations. Because of this unconventional form, new methods of calculating control laws (which can operate in real-time) need to be developed. Control laws of various types that exploit characteristics of the system structure should probably receive the most attention in sponsored research.

Large-scale systems, by virtue of their size, also make the diagnosis of fault/failure conditions extremely difficult. In a manufacturing facility, the goal of process control is to maintain product quality under safe operating conditions; the minimization of energy consumption is a parallel concern that can also be a primary goal. When operating conditions fall outside of acceptable design limits, because of equipment malfunctions and/or human errors, product quality deteriorates, energy consumption becomes non-optimal, and unsafe conditions may prevail. Such excursions may require plant shutdown or may lead to catastrophic events such as explosions, fires, or discharge of toxic chemicals. In most existing control systems, abnormal measurements trigger alarms that alert the process operator. The operator then must take remedial action to either return the plant to normal levels of operation or shut the facility down.

The success of a manual strategy for handling abnormal conditions relies very heavily on the operator's correct

response to process alarms. However, the operator's response depends on many factors: the number of alarms and the frequency of occurence of abnormal conditions; the man-machine interface and how information is presented to the operator; the compexity of the plant (which might be influenced by energy-conserving designs as well as by complex control strategies); and the operator's intelligence, training, experience, and reaction to stress.

Many factors are involved in determining the appropriate response to an alarm situation and are influenced by the fact that the alarms interact because of the presence of feedback control loops. Thus, computational aids for the operator are crucial to the success of the operation of complex, large-scale manufacturing plants. Such computational aids may be developed as rule-based software systems, called *expert systems*, since they are based on emulating the actions of a human expert who can perform the required tasks at a high level of proficiency.

One of the important uses for expert systems in the field of control theory is in fault diagnosis, namely, to develop algorithms and software systems for assisting the plant operator in dealing with plant upsets. The terms fault, failure, and malfunction have many connotations in the literature as well as in general usage. Here, the words *fault* and *malfunction* in relation to equipment are synonyms that designate the departure from an acceptable range of an observed variable or calculated parameter associated with the equipment. *Failure*, on the other hand, means the complete inoperability of equipment or the processes. That is, the equipment or an instrument lacks the capability of carrying out its specified funciton.

If more than one cause of a fault can occur, *fault diagnosis* refers to the determination (after detection of the occurrence of a fault) of the equipment, or portion thereof (subsystem) that is causing the fault(s). Because of the interaction among process components, it is very difficult to isolate causes that occur in complex systems. The engineer or operator wants to obtain the maximum possible degree of discrimination, using the available test data, with the least amount of computation.

The degree of difficulty of fault detection and diagnosis depends very much on the nature of the fault. Complete malfunction of a piece of equipment is usually relatively easy to detect, but by the time it has occurred, considerable damage may have taken place. Detection of incipient or latent malfunctions, or process degradation, is more difficult, although perhaps more important. A fault detection system should respond rapidly when a fault or malfunction occurs. On the other hand, the system can then become too sensitive to noise, and consequently may generate too many false alarms. However, it is more reasonable to tolerate false alarms in a highly redundant system configuration than in a system without substantial back-up capabilities. Another trade-off involves the complexity of the detection (measurement) system, and hence its expense relative to its performance. By examining specific forms of process behavior that are characteristic of certain faults or malfunctions, one should be able to reduce the fraction of false alarms as well as any missed faults by making simultaneous multiple measurements.

Many questions need to be resolved by further research:

(1) What are good on-line diagnostic procedures? Can they be based upon measurements, where the process variables are within allowable limits rather than in extreme stress?

(2) If such procedures exist, how can they be implemented economically in practice? What is the role of process simulators in developing such procedures?

(3) Under what circumstances can the causes of faults be included in the mathematical models of the instruments?

(4) What properties of system structure and behavior are conducive to on-line diagnosis?

IV. Potential Payoffs

It is difficult to estimate the potential payoff for improved technology in the systems, instrumentation, and control area, either as energy or money saved. However, the interdisciplinary nature of the technology gives it very broad applicability in the energy industries.

Sensors are particularly important to energy exploration and production. Exploration and production costs represent a significant fraction of the cost of fuel delivered to the user. This is particularly true in the case of new finds, which may be quite deep, far offshore, or located in hostile environments. Sensor systems that can locate oil, gas, uranium or other fuel sources faster, deeper, more reliably, or in smaller quantities, would increase the domestic reserves of U.S. fuel sources as well as make them available at lower cost. Increased production/recovery efficiencies for fuels such as oil, shale or coal would be obtained with advanced instrumentation.

Improved sensors can also have a significant impact on the efficiency of various processes for energy delivery and conversion. In the field of internal combustion engines, distinct gains (perhaps leading to absolute increases of 5% to 10% in gasoline economy)

could be achieved through more comprehensive sensor systems. The efficiency of stationary combustion systems could also be improved, although the incentive is probably not as great. In addition, more precise control of air pollutants could be achieved with improved instrumentation of combusion systems, without sacrificing power conversion efficiencies.

Improved control theory (Area B in Table 1) can also improve energy usage and efficiency in various processes. This can be done by reducing product variability and eliminating products below market specifications.

Improved control and simulation tools and software (Area C) may have the largest impact in discrete manufacturing systems and batch processes. This is because the typical discrete manufacturing or batch plant is a multipurpose plant, where the processing sequence for each product is quite distinct. The scheduling problems associated with such systems are challenging and involve complex combinatorial optimization problems, which are currently solved in a non-optimal fashion. Energy savings from improved analysis methods could be significant. Potential applications exist in discrete parts fabrication as well as in the pharmaceuticals, biotechnology, and microelectronics industries.

The use of artificial intelligence and expert systems to deal with large-scale processes (Area D) is in its infancy. In a large processing plant, there may be several thousand measurements and alarms that need to be monitored by the operator. The operator must decide which measurements/alarms are accurate and which ones are spurious. An expert system would provide assistance to the operator to deal with such problems. Savings in energy usage here would arise by

reducing the periods of time when the plant is not functioning properly (or manufacturing an unsatisfactory product). Other applications of this technology could include the rectification of fouled measurement instruments in coal conversion plants and detection or control of natural gas leakage in pipelines.

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How to get your Paper Accepted for Presentation at an AIChE Meeting

Bruce A. Finlayson, University of Washington, Former 10a Chairman, Current Director of CAST

Your pet project has come to fruition and you would like to share the results with the profession. How can you get your paper accepted for presentation at an AIChE meeting? Eventually your paper will be judged on its merits, but before that point there are steps that you can take to maximize your chances. Here they are.

Your paper can only be presented in a session of related papers. Are there such sessions planned? Yes, there probably are. The trick is to find them. As a member of CAST you have people working for you: the programming board plans 2-3 years in advance and the CAST Newsletter gives those plans to you (see Meetings and Conferences section). Look at the list of future sessions and decide which sessions are related to your paper. If you do not find one, maybe there needs to be one. To help create a session you can (a) write the area chairman and suggest subjects for a future meeting, (b) attend the 10a-10c program meetings at an AIChE meeting, or (c) volunteer to be a session chairman. At the fall meeting, Area 10a meets at noon on Tuesday, Area 10b meets at 5:30 p.m. on Wednesday (tentatively), and Area 10c meets at noon on Wednesday. Find the room by getting a list of meetings at the AIChE registration desk. Hopefully the programming board is sufficiently on top of the work going on that several pertinent sessions already exist.

Suppose you have identified possible sessions that match your paper. What do you do next? Contact the session chairman and indicate interest in presenting a paper. He will send you session announcements and indicate the dates for submission of abstracts. You may be surprised by the long lead time, which is a result of various AIChE policies. While such a situation may change, today it is a fact of life. Thus, for a paper at the fall annual meeting, you need to present an abstract in January. The session chairman makes his decisions about February 1. For the spring meeting, the session chairman may need to make a decision about July 1. This is why it is very important to pick sessions far in the future. The earlier you let the session chairman know, the better are your chances. The session chairman then has a better idea of the demand for his session and this gives him data to use in preventing the meeting program chairman from cancelling your session. If the demand is great enough, and is known far enough in advance, perhaps even more sessions can be offered.

One thing is clear: do not depend on CEP for submitting your paper. By the time you see the sessions listed in CEP there is very little time for you to submit your paper. Rather, use CEP for decisions about whether to attend the meeting. Use the CAST newsletter to decide where to present the paper–the sessions are listed there far in advance. In fact, by using information in the CAST newsletter, you can look at meetings two years in advance and even orient your project to help it fit into a future session. Let's see how this works.

Suppose you are working on the use of expert systems to design control systems. Look at the future sessions for the New York meeting (see Meetings and Conferences section in this newsletter). It is possible that your material could be included in the session entitled Design and Control or the session entitled Expert Systems. The session chairman needs the abstract by February 1, 1987. Consequently it is time now to begin to get company clearance for publication.

In summary, to give your paper its best chance:

(1) pick session(s) at least a year in advance;

(2) write the session chairman to indicate interest;

(3) submit your abstract by the session deadline, which will be very early.

As a CAST member, you can thank the programming board and the editor of the newsletter for making the needed information available to you far in advance of the meeting.

Good luck.

Systems Research at The University of Maryland, College Park

Thomas J. McAvoy, University of Maryland

In the summer of 1984 the National Science Foundation announced a new program to support centers of excellence. One of the goals of the new centers was to focus research efforts in areas that could make the United States more competitive economically. These areas typically involve complex problems where interdisciplinary cooperation is a necessity for progress. Another novel aspect of the program is

that the education of both graduate and undergraduate engineers in the focus area of the center had to be addressed in the proposal. In essence, NSF wanted to ensure that developments made in the centers filtered out to industry via the students graduating from the host institutions.

The University of Maryland was selected as one of the six initial awardees; the Center is called the Systems Research Center (SRC). The Systems Research Center has as its focus three technology drivers: (1) artificial intelligence, (2) computer-aided design, and (3) VLSI circuitry. The goal of the Center is to study the impact of these drivers on five application areas: chemical process control, flexible manufacturing, communications, stochastic systems, and servomechanism design. Included in the flexible manufacturing area is work on robotics being carried out at Harvard University, which is a sister institution for the research.

The University of Maryland has committed 12 additional half-time faculty positions for the SRC; three of these are in the chemical process control area. A total of seven full-time chemical engineering faculty are working on SRC-supported research. A number of broad project areas in chemical process control are being investigated. These include the application of artificial intelligence to control system analysis and design, process alarming, and knowledge extraction from process operators; modeling, control, and optimization of polymer and biochemical reactors; on-line process identification and optimization; and control system robustness. Through SRC funding, a new 2 x 2 Lambda Plus Artificial Intelligence computer has been purchased from Lisp Machines for use by the chemical process control group.

In addition to the research to be carried out in conjunction with the SRC, the process control group at Maryland has also established ties with the Chemical Process Metrology group at the National Bureau of Standards. This group carries out research on a variety of measurement techniques of importance in process control. The NBS and SRC interaction provides the process control group at Maryland with a truly unique capability. The SRC faculty are particularly strong in optimization and control theory, while the NBS personnel are experts in the area of process measurement. A research team with this broad a range of expertise is unique in the U.S. and abroad.

For additionaql information on chemical process control research at the University of Maryland, please contact Dr. Thomas McAvoy, Department of Chemical Engineering, University of Maryland, College Park, MD 20742, (301) 454-4593.

Carnegie Mellion's Engineering Design Research Center

Georgette Demes, Assistant Director

A new NSF Engineering Research Center was established at Carnegie Mellon in May of 1986. Known as the Engineering Design Research Center (EDRC), its goal is to develop ways to design products much better and faster. Research scope covers all stages of a product's life including manufacture, testing, maintenance, and disposal.

Co-Directors of the EDRC are Arthur W. Westerberg, Swearingen Professor of Chemical Engineering, and Sarosh N. Talukdar, professor of electrical and computer engineering. Westerberg and Talukdar work closely with a network of affiliated Carnegie Mellon faculty and graduate students from Chemical, Civil, Mechanical, Metallurgical and Electrical Engineering, as well as Architecture, Computer Science, Mathematics, Psychology, the Graduate School of Industrial Administration, and Engineering and Public Policy. The EDRC staff comprises administrative personnel and research enginers.

Since industry is the place where design problems originate and where their solutions are tested, EDRC invites industry to tak an active part in its research activities. Various forms of industrial involvement are available. These include participation in planning, equipment selection, visitor exchanges, and an industrial affiliates program.

EDRC researchers are currently exploring five areas:

- Synthesis–to understand and develop automatic techniques for the generative aspects of design.

- Design for Success in Manufacture, Maintenance, and other 'Downstream Concerns'–to develop techniques for coordinating the various design stages in a product's life cycle and ensure that the product can be manufactured, tested, used, and so forth.

- Tool Integration–to develop systems that can produce prototypes in a tenth or less of the time required by conventional approaches.

- Design Styles–to study how design is done in different industries and countries.

For those who desire more information, please call (412) 268-2229 or write to the Engineering Design Research Center, Carnegie Mellon, Doherty Hall A219, Pittsburgh, PA 15213.

Microcomputer/Personal Computer Notes

Peter R. Rony

Business Computer Systems (October 1985) briefly summarized progress on linguistics software, one of the faster growing niche markets in office automation (100 to 250 percent increase per year). Both ALPS and Weidner Communications Corp. have introduced IBM AT- and XT-based translations systems. Their cost is still high, $19,000 and $10,000, respectively, but is certain to decline significantly within five years. The same issue contains information on *"Bridges and Gateways"* between local area networks, high-quality graphics software, and three macro processors (Keyworks, SuperKey, and ProKey 4.0).

Byte's 10th Anniversary Issue (September 1985) had homebrewing as a theme. An article that caught your editor's eye, as a long-time 8080A/8085/Z80 microprocessor user, is *"Build the SB180 Single-Board Computer,"* by Steve Ciarcia. The single-board 8-bit processor is based upon the Hitachi CMOS Z80-code-compatible processor, HD64180, which directly addresses 512 kbytes and has a number of important hardware goodies built into the 64-pin chip. The message that engineers should keep in mind is that the two major 8-bit family microprocessors (8080A and 6502) continue to thrive in tens of thousands of products that do not require 16-bit processors. By the end of the decade, a gallium arsenide Z80-family microcomputer should become commercially available that has a clock speed in excess of several hundred megahertz.

The September 1985 issue of Byte also contains *"A Microcomputer Timeline"* that summarizes key dates in the history of microcomputers starting with 1974. Not widely appreciated these days is the modest role that a small university town in Virginia–Blacksburg–played in the early days of homebrew microcomputer systems and microcomputer education. Included in the timeline is the July 1974 issue of Radio-Electronics, *"Build the Mark-8, Your Personal Computer,"* developed by a Blacksburg chemistry graduate student, Jon Titus. Jon also developed the first microcomputer trainer, the MD-1, which was introduced in the summer of 1975 and incorporated solderless breadboarding techniques. The first university-originated textbook on microcomputers was published in Blacksburg in August 1975.

Need to construct a parallel-to-serial printer port adapter for your laboratory computer? See the article by Howard Austerlitz in the September 1985 issue of Byte, pages 257-260. Mark Hanslip shows you how to *"Add Function Keys to Your Microcomputer,"* pages 263-268.

The October 1985 Computer, a publication of the IEEE Computer Society, is a special issue on computer-based multimedia communications. Articles focus on the electronic book, real-time conferencing systems, office document interchange formats, graphics standards, the DARPA multimedia mail systems, and a distributed interoffice mail system. *"Computer Conferencing"* is the subject of a series of nine articles in the December 1985 issue of Byte magazine.

"Telecommunications Standards Arrive" (pages 84-96 in the October 15 issue of Datamation) provides a provocative quote from J. A. N. Lee: *"One quarter of the total available computer power in the U.S. is being used to provide conversion systems between dissimilar, nonstandardized (or nonstandard) elements of computer systems."* The quote dates back to 1976, but apparently is valid today.

Dr. Dobb's Journal (September 1985) describes *"Two TEX Implementations for the IBM PC"* (pages 80-91). TEX is a system for typesetting technical text developed by Donald Knuth. The October 1985 issue of Dr. Dobb's is dedicated to *"The Future of Forth;"* the characteristics of the Novix NC4000 processor, a threaded-code hardware microprocessor for the Forth language, are given. Specialized microprocessors designed for the execution of high-level languages–NC4000, Forth Engine, H.Forth, CLM, Spur, Soar, X-1, and ACAPS–are summarized in the February 6, 1986 issue of Electronic Design (pages 26-32). Electronics magazine (November 25, 1985, pages 58-60) also treats this topic. Consider LISP-on-a-chip for AI applications in small computers and products that contain embedded microcomputers.

New computer jargon: *silicon supermarket*, which is defined as a chip fabrication company that can supply developers with all their computer-aided engineering needs under one roof.

Volume 10, Number 11 of Byte, a special IBM issue, contains several items of interest: (a) An editorial on Intel and Future IBM PCs, the iAPX286/386, and the Motorola MC68000; (b) An annotated bibliography of recent books on the IBM PC family (pages 11-35); (c) Public-domain utilities for the IBM PC (pages 39-54); (d) A discussion of important differences between the 8088 and 80286 microprocessors (pages 93-101); (e) Programming suggestions on the writing of desk accessories (pages 105-122); (f) Benchmarks of IBM PC clones (pages 195-201); and (g) IBM PC-family BIOS comparisons (pages 259-265).

Digital signal processors will be the subject of a presentation at the Annual AIChE Meeting in Miami Beach; new

DSP chips are described in the August 26, 1985 issue of Electronics (pages 42-46).

The November 1985 issue of Byte magazine provides extensive hardware and software (BASIC) details about the XECOM XE1203 MOSART module, "The World's Smallest 1200-bps Modem" (pages 89-108). In the same issue, Mark Bridger and Mark Goresky show you how to produce "High-Resolution Printer Graphics" (pages 219-232) by addressing the individual dots used to generate printed dot-matrix characters.

Ralph Levien, in the February 1986 issue of Byte, describes a LISP editor that lets you create LISP programs visually ("Visual Programming," pages 135-144). Golden Common LISP, a variant of Common LISP, which is "a standard LISP blessed by the Department of Defense" is reviewed in the December 1985 Byte (pages 317-321). Grapes is the name for Advanced Computer Tutoring's AI-based system for learning LISP (Electronic Design, November 28, 1985, page 38).

Ten programming editors/programmable editors for MS-DOS are compared from the standpoint of features, size, documentation and help, editing commands, search and replace, file and window management, text formatting commands, printing, undo, keystroke macros, macro language, subprocesses, error handling, benchmarks, miscellaneous features, and overall evaluation in the November 1985 issue of Dr. Dobb's Journal. The difference between Modula-2 and Pascal for microcomputers is also discussed.

An elegant way to bring up a 68000 microcomputer as a free-running system is described by Alan D. Wilcox in the January 1986 issue of Dr. Dobb's Journal (pages 60-74). Excellent block diagrams, schematics, and timing diagrams are provided. The article may be useful for those hardy souls who are working with 68000-based laboratory computer systems.

Have you ever wondered what a cyclic redundancy check (CRC) does in detecting errors in data transmission? If so, you should read "The Great CRC Mystery," by Terry Ritter in the February 1986 issue of Dr. Dobb's (pages 26-34).

Project-management software is the focus of a product report in the December 12, 1985 issue of Electronic Design (pages 149-158). Forty-two products are included in the published directory.

A glimpse at future developments in microelectronics technology can be obtained by studying the 1986 Technology Forecast published in the January 9, 1986 issue of Electronic Design. The 50 to 200 chips on a single printed circuit board will be consolidated, in several years, into several large VLSI integrated circuits. Some of the articles are on software tools for IC design, electronic breadboarding, analog standard cells, programmable logic devices, and a silicon compiler tool set.

The feature article in the January 23, 1986 issue of Electronic Design (pages 73-82) is the Texas Instruments TMS34010 32-bit CMOS graphics processor. It uses a 6 million instructions per second (6 MIPS) general-purpose instruction set and special pixel-processing instructions and handles bit-mapped graphics.

The one-chip modem is described in the November 5, 1985 issue of Electronics (pages 46-52), making it easier to build modems into a variety of products that require serial communications.

For $95, you can purchase "Pocket APL," an inexpensive yet complete version of the language for an IBM PC.

Details and benchmarks are given in the March 1986 issue of Byte (pages 237-243). "68000 Wars: Round 1" between the Macintosh, Amiga, and Atari 520ST are discussed by Bruce Webster in the same issue (pages 305-322).

Do ASCII-based communications have a future relative to more advanced protocols such as IBM's Systems Network Architecture (SNA) protocols? The question is discussed by Michael Tucker in the November 1985 issue of Mini-Micro Systems (pages 119-124).

Curious how a windowing environment manages memory? PC Magazine treats GEM Desktop, Microsoft Windows, TopView, and DESQview in the February 25, 1986 issue (pages 108-132). I vowed not to worry about word processors anymore in this column, but must mention the extensive discussion of new products by John Dickinson in the same issue (pages 177-214).

"CAD: The Big Picture for Micros," is the cover story of the March 11, 1986 issue of PC Magazine (pages 108-180). A major series of article. "The IBM Token-Ring LAN: What? Why? Now?" appears in the same issue. In the March 25, 1986 issue of the same magazine, the IBM Enhanced Graphics Adapter (CGA) standard and color monitors are featured (pages 108-144).

A hint at the future: parallel-processing engines (Electronics, November 18, 1985, pages 23-24). Two companies are preparing hardware that will turn an IBM PC AT into a multiple-processor parallel engine. ITT's massively parallel Personal Supercomputer Co-processor, slated for a 1987 debut, is expected to handle 120 million 32-bit floating-point operations per second and provide 100 Mb/s of external I/O bandwidth.

Read about "Optical ICs: The New Alternative" in the November 18, 1985

issue of Electronics (pages 39-44). The bulk of R and D has focused on integrating optical components, constructing optoelectronic components that combine electronic and optical logic elements onto the same monolithic substrate, and fabricating vertical superlattice structures.

In the *"Battle of the Buses: And the Winner Is . . . "* (Electronics, November 25, 1985, pages 48-51), the Motorola/Mostek/Signetics 32-bit VME hardware bus has a three-year head start over the Intel 32-bit Multibus II. For 8- and 16-bit systems, Intel's Multibus I has been dominant.

The December 23, 1985 issue of Electronics has several stories on VLSI analog chips, which are following in the footsteps of digital VLSI, and *"The Big News at ISSCC: Digital Signal Processors."* An article by Bernard Conrad Cole (pages 50-52) summarizes developments in analog technology, signal processors, general-purpose processors, semicustom ICs and arrays, and memories presented at the International Solid-State Circuits Conference in February 1986. IBM has a 32-bit single-chip microprocessor that incorporates 102 mainframe instructions and supports emulation of the rest of the instruction set. The followup article in the February 17, 1986 issue of Electronics (pages 23-31) describes these developments in greater detail. More on ISSCC–digital chips, analog chips, and special-purpose chips–is contained in the February 20, 1986 issue of Electronic Design.

A *"smart analog IC"* is a semiconductor circuit in which the analog and digital worlds have been merged. Analog operations occur under the watchful control of digital logic. See Electronics, January 20, 1986, pages 21-22.

"Slamming the Door on Data Thieves" (Electronics, February 3, 1986, pages 27-31) presents some tutorial information on different forms of data encryption, including cipher-block chaining, cipher feedback, and output feedback.

A favorite annual special issue is the *"Technology '86"* issue published in IEEE Spectrum (January 1986). Fields covered include minis and mainframes, personal computers, software, microprocessors, communications, solid state, instrumentation, industrial electronics, power and energy, consumer electronics, transportation, aerospace and military, medical electronics, and specialties.

Forum

Do chemical engineers have opinions, suggestions, ideas? We would very much like to receive comments from the CAST Communications readers. Even though the publication frequency precludes rapid dialog, your input could be of interest to our readers. The best brief notes we receive will be published in the next edition of CAST Communications.

The Editors

Meetings and Conferences

The following items summarize information in the hands of the Editor by September 22, 1986. Please send CAST Division session information, meeting, and short course announcements to me by February 15, 1987 for inclusion in the spring 1987 issue of CAST Communications.

Peter R. Rony,
Editor, CAST Communications

Foundations of Computer Aided Process Operations
(FOCAPO)
July 5-10, 1987
Park City, Utah

The objective of this one-week specialist conference is to provide an in depth review of the state-of-the-art, general problems and research needs in the area of computer-aided plant operations. The structure of the conference will parallel that of the CPC (Control) and FOCAPD (Design) conferences. Specifically, it will involve a limited number of invited speakers and commentators, ample periods for discussion by the participants, a single contributed paper session organized in a poster session format, and a restricted number of attendees.

Program

The program of the meeting is nearly finalized and consists of the following sessions, speakers, and commentators.

Process Data Acquisition and Interfaces (Dr. John Hale, DuPont, chairman and Dr. Patrick Kennedy, Oil Systems Inc., commentator)

"Plant Scale Process Monitoring and Control Systems," by Lawrence DeHeer, Engineering Department, DuPont

"Data Screening," by Prof. Richard Mah, Northwestern University

Process Safety (Prof. Gary Powers, Carnegie Mellon University, chairman; Malcom Preston, ICI, co-chairman; and Prof. P. Andow, Loughborough University of Technology, commentator)

"Systems Engineering Issues in Process Safety," H. A. Duxbury and M. L. Preston, ICI PLC

"Human Factors in Process Operation Safety Analysis: The Computer/Human Interface," by William Brasie, Dow Chemical

"Probabilistic Risk Assessment," by Prof. Gary Powers, Carnegie Mellon University

Operations Planning (Prof. David Rippin, E.T.H. Zurich, chairman; Tony Perris, Air Products UK, co-chairman; commentator to be confirmed)

"Application of OR Methodology to Process Operations," by Charles White, DuPont

"Supply Chain Management in the Packaged Food Industry," by B. A. Sigrist, Nestle SA, Vevey, Switzerland

Maintenance Planning (Tony Perris, Air Products UK, chairman; Prof. David Rippin, E.T.H. Zurich, co-chairman; and Frank Pierce, Union Carbide, commentator)

"A Systems Engineering Approach to Reliability, Availability, and Maintenance," by C. F. H. Van Rijn, MSE Dept., Shell Research, Amsterdam

"Systems Approach to Maintenance Planning," Terry W. Williams, Stearns Catalytic Corp.

Process Simulation (Rufus Baxley, Union Carbide, chairman; Prof. Jack Ponton, University of Edinburgh, commentator; and Edward M. Rosen, Monsanto Co., commentator)

"Modeling and Simulation in Process Operations," by J. D. Perkins, G. W. Barton, and R. M. Pitblado, University of Sidney

"A Block Structured Approach to Dynamic Process Simulation," by Toshi Shinohara, C. E. Simcon

"Equation Based Process Simulation," by R. F. Preston and G. B. Gochenour, Shell Oil Company, Houston

Process Optimization (Prof. Ignacio Grossmann, Carnegie Mellon University, chairman; David R. Heltne, Shell Development Co., commentator; and Jerry L. Robertson, Exxon R and D, commentator)

"Large Scale Mathematical Programming Systems for Process Operations," by John Tomlin, Ketron Inc.

"Optimal Redesign and Modification of Existing Plants," by Prof. Arthur Westerberg, Carnegie Mellon University

Plant Networks and Data Bases (Dr. Norm Rawson, IBM, chairman and Prof. D. Grant Fisher, University of Alberta, commentator)

"Plant Information Networks," by John Heafner, National Bureau of Standards

"Manufacturing Databases in Distributed Environments," by Wil Plouffe, IBM Research

"Plant Data Management: Practice and Futures," by Charles H. Reese, Chevron Corporation

Intelligent Systems in Process Operations (Prof. George Stephanopoulos, MIT, chairman and Brian Matthews, Exxon Chemicals, commentator)

"The Scope of Artificial Intelligence in Plant-Wide Operations," by Prof. George Stephanopoulos, MIT

"Expert Systems for Process Fault Diagnosis: A General Framework," by Prof. Mark Kramer, MIT

"Evaluation of Experience with an Expert System for Fault Diagnosis in a Commercial Scale Chemical Process," by Profs. D. E. Lamb, D. Chester, and P. Dhurjati, University of Delaware

Poster Session: Innovative Research in Process Operations (Prof. J. Douglas, University of Massachusetts, chairman; rapporteur to be confirmed)

The poster session, consisting of a limited number of contributed papers, will be held on Thursday afternoon (July 9). Authors interested in contributing a paper to this session should submit a title and two-page abstract to the session organizer, Professor James Douglas, Dept. of Chemical Enginering, University of Massachusetts, Amherst, MA 01003, by January 1, 1987.

Conference Site

The conference will use the facilities of the Prospector Square Hotel, which has both a fully equipped Conference Center and a complete Athletic Club. Acommodations include hotel rooms, studios as well as condominiums. Common breakfast and dinner services are planned at a cost. Park City, Utah, is a summer/winter mountain resort originally founded as a silver mining camp. The Park City area offers mountain hiking and horseback riding, tennis, golf, bicycling, ballooning and gliding as well as water sports at one of three reservoirs located within 25 minutes drive. As the largest resort community drive in Utah, Park City has interesting shops and boutiques, art galleries, and summer theater for the less athletically inclined. The town is 40 minutes by car from the Salt Lake City International Airport and is served by airport limos. The Salt Lake City area is within a few hours drive of famous national parks such as Yellowstone, Zion, Bryce, Arches, the Grand Canyon, and Lake Powell.

Application Form for Participants

Attendance at the FOCAPO Conference will be limited, and is by invitation following receipt of an application form. Requests for application forms should be directed to the CACHE Office, P.O. Box 7939, Austin, TX 78713-7939. The deadline for the submission of applications is **January 15, 1987**. Selection of attendees will be made on the basis of involvement and experience in the field of computer-aided process operations. Notifications of selection will be issued by March 15, 1987.

For further information about the technical program, inquiries should be directed at the Conference Chairs:

G. V. Reklaitis
School of Chemical Engineering
Purdue Univ.
W. Lafayette,
IN 47907

H. Dennis Spriggs
Linnhoff-March U.S.A.
P.O. Box 7577
Charleston,
WV 25356.

Area 10c Committee Meeting
(April 9, 1986)

The FOCAPO conference, scheduled for August 1987, is moving ahead on schedule. NSF funding request will be presented in May, and the agenda and speakers will be finalized by the end of April. A request to the Programming Board will be made for additional CAST sessions starting with 1987 meetings. A fourth CAST section was suggested. "CAST programming would be divided into:

- 10a Systems and Process Design

- 10b Systems and Process Control

- 10c Operations and Information Processing

- 10d Analysis"

"The intent of the reorganization is to provide a forum for the mathematically oriented papers which have been grouped with design and to focus 10c on the plant operations area, which is of high interest today. No action was taken but discussion implied a commitment to this organization in 1987 if no one objected." Reactions to the reorganization suggestion are solicited. Please send them either to the CAST chairman or the editor.

1986 AMERICAN CONTROL CONFERENCE, SEATTLE
(June 18-20, 1986)

For those of you who did not attend this conference, here is a brief listing of the papers in the sessions that were organized by the AIChE society review chairman. Details of author affiliation can be obtained from the official conference program, a copy of which is in the possession of Yaman Arkun, the AIChE society review chairman. His address is School of Chemical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0250, (404) 894-2871.

Session WA1. Robustness and Modeling Issues in Process Control

"Synthesis of the IMC Filter by Using the Structured Singular Value Approach," by Zafiriou and Morari

"Spectral Radius Design for Robust Multivariable Control," by Kantor

"Refined Block Relative Gain and its Role in the Design of Robust Decentralized Control," by Arkun and Manousiouthakis

"Prudent and Robust Self-Tuning Regulators," by Sela and Ray

"Impact of Modeling Decisions on the Robustness of Tubular Chemical Reactors," by Palazoglu and Owens

"The Equivalence of Non-Interacting Control System Design Methods in Distillation," by Bequette and Edgar

Session WA5. Artificial Intelligence in Process Control

"Use of Expert Systems in Closed Loop Feedback Control," by Arzen

"Expert System Rules from CAD Databases," by Beazley

"An Artificial Intelligence Approach to Assembly Line Trouble Shooting," by Kahn

"Performance Analysis of Real-Time Expert System Tools," by Leah and Sinnamohideen

"Towards an Expert Control Designer," Jacobs and Antsaklis

"Application of Intelligence to Chemical and Biochemical Process Supervision Systems," by Visuri and Karim

Session WP1. Advances in Model Predictive Control

"A Contraction Mapping Analysis of Stability and Robustness Properties of Model Predictive Control," by Reid, Mahmood, and Mehra

"Infinity-Norm Formulation of Model Predictive Control Problems," by Morari and Campo

"Adaptive Horizon Adjustment for Model Predictive Control," by Brosilow and Quigley

"Microprocessor-Based Surge Level Control," by Stewart and Lau

"Model Predictive Control of Gas Pipeline Networks," by Marques and Morari

"*Predictive Control of Multi-effect Evaporation System*," by Ricker, Sim, and Cheng

Session TA1. Recent Developments in Process Control

"*Application of Singlar Value Decomposition to the Design, Analysis, and Control of Industrial Processes*," by Moore

"*Improvements in Compartmental Modeling for Distillation*," by Horton, Bequette, and Edgar

"*The Mu Interaction Measure*," by Grosdidier and Morari

"*Disturbance Rejection Through Model Dependent Control*," by Svoronos

"*Predictive Control Using Observers for Load Estimation*," by Yuan and Seborg

"*A Predictive-Based Multivariable Controller for Processes With Distinct Time Delays*," by Park and Clough

Session TA3. Adaptive Process Control

"*Adaptive Inferential Control*," by Brosilow and Pollard

"*Adaptive Inferential Control for Chemical Processes with Limited Measurement Problems*," by Lee and Shen

"*Robust Adaptive Control in the Presence of Unmodeled Dynamics*," by Shah, Cluett, Fisher, and Martin-Sanchez

"*A Comparison of Long Range Predictive Control With GMW and LQG Regulators in a Highly Nonlinear Environment*," by Morris, Montague, and Tham

"*On-Line Estimation of Time Delay and Continuous-Time Process Parameters*," by Agarwal and Canudas

"*On-Line Adaptive Optimal Control*," by Petersen and Whyatt

Session TP1. Nonlinear Process Control

"*Nonlinear State Feedback Synthesis by Global Input/Output Linearization*," by Kravaris

"*Nonlinear Heat Exchanger Control Through the Use of Partially Linearized Control Variables*," by Edgar and Alsop

"*Stability of State Feedback Transformations for Nonlinear Systems*," by Kantor

"*Nonlinear Control of an Exothermic CSTR*," by Cinar, Rigopoulos, Shu, and Meerkov

"*Control Stategies for Nonlinear Multivariable Systems with Time Delays*," Seborg and Wong

"*Nonlinear Control Structures for Chemical Reactors*," Bartusiak and Georgakis

"*Nonlinear Inferential Control of Reactor Effluent Concentration from Temperature and Flow Measurements*," by Brosilow and Parrish

"*Nonlinear Internal Model Control*," by Economou and Morari

Session TP6. Simple vs. Complex Models in Process Controls

"*The Hierarchy of Models in Chemical Process Control*," by Pearson

"*Statistically Derived Static Process Models*," by McClure

"*Cluster Analysis and Lumpability of Large Linear Systems*," by Coxson

"*Low Order, Nonlinear, Dynamic Models for Distillation Columns*," by Wong and Seborg

"*The Value of Simple Multivariable and Nonlinear Models in Process Control*," by Georgakis

"*Remarks on Stochastic Model Reduction*," by Zhóu and Khargonekar

Session FA1. Applications of Advanced Process Control. I

"*Predictive Control Based on Constrained Optimal Control*," by Edgar and Little

"*Achieving Decoupling with Predictive Controllers*," by Mellichamp, Seborg, and Maurath

"*Synthesizing a Multivariable Predictive Algorithm for Noninteracting Control*," by Deshpande, Arulalan, and Chawla

"*Robust Controller Design for a Fixed-Bed Methanation Reactor*," by Morari, Mandler, and Seinfeld

"*Theoretical and Experimental Results on an Efficient Method fór the Design of More Effective Dynamic Decouplers and Feedforward Compensators*," by Ogunnaike, Nelson, and Tuttrup

"*Vibrational Control of an Exothermic CSTR*," by Cinar, Rigopoulos, and Meerkov

Session FP1. Applications of Advanced Process Control. II

"*Short-Cut Analysis of Pressure Control in Steam Headers*," by McAvoy and Bertrand

"Control of Recombinant Escherichia coli With Temperature-Sensitive Plasmid pOU140," by Dhurjati and Galt

"Experimental Application of Advanced Strategies to Transverse Thickness Control of Extruded Webs," by Leffew

"On-Line Estimation of Molecular Weight Distributions in Methyl Methacrylate Polymerization," by Taylor, Gonzalez, and Jensen

"The Hyperplane Algorithm Used in Continuous Kinetic Processes," by Bozenhardt

"Modeling and Control of a Copolymerization Reactor," by Congalidis, Richards, and Ray

Miami Beach AIChE Meeting
(November 2-7, 1986)

Area 10a Sessions

1-2. **Applied Mathematics I and II.** Lyle Ungar (Co-Chairman), Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 19104, (215) 898-7449 and Stuart W. Churchill (Co-Chairman), Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 19104, (215) 898-5579. Papers in Session I include:

"Rate Process Based Continuation Applied to Hydrometallurgical Solvent Extraction," by Frantz and Van Brunt

"A Numerical Study of Global Bifurcations in Chemical Dynamics," by Kevrekidis

"Second- and Third-Order Resonance Phenomena in Three-Dimensional Oscillating Drops," by Natarajan and Brown

"Application of a Specialized Approximating Function in the Numerical Solution of Chemical Reactor Models," by Chiu and White

"Numerical Resolution of Front Phenomena by Regridding Techniques," by Degreve, Kimitriou, Puszyuski, and Hlavacek

"Waveform Methods for Solution of Large Systems of Stiff Differential Equations," McRae

"Propagation Phenomena in Nonsteady-State Continuous Counter-current Processes–An Analytical Application of Method of Characteristics," by Hwang

Papers in Session II include:

"Boundary Integral Element Analysis of Conduction Through Dense Dispersions," by Durand and Ungar

"The Kinetic Theory of Fragmentation," by Ziff and McGrady

"Uniqueness of Solutions to Isobaric Flash Processes Involving Homogeneous Mixtures," by Lucia

"Self-Adjoint Operators in Interacting Solid-Fluid Systems Transport in Packed Bed," by Arce and Ramkrishna

"Identification of Spatially Discontinuous Parameters in Second-Order Parabolic Systems," by Chung and Kravaris

"Optimization of Differential-Algebraic Systems," by Curthell and Biegler

"Pricing Theory and the Resolution of Multi-Objective Tradeoffs," by Stephanopoulos and Doldan

3-5. **Simulation in Chemical Engineering** I, II, and III. Arthur W. Westerberg (Co-Chairman), Department of Chemical Engineering, Carnegie-Mellon University,

Pittsburgh, PA 15213, (412) 268-2344 and Warren D. Seider (Co-Chairman), Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA 19104, (215) 898-7953. Papers in Session I include:

"Adaptive Finite Element Simulation of Stagewise Separation Processes," by Swartz and Stewart

"A Design Procedure for Distillation Columns with Non-Sharp Splits," by Levy and Doherty

"Heterogeneous Azeotropic Distillation–Simulation Using Homotopy Continuation Methods," by Kovach and Seider

"Simulation of Azeotropc and Extractive Distillation Operations Using a Nonequilibrium Stage Model," by Powers, Vickery, and Taylor

"Alambic–A Vectorized Batch Rectification Simulator Running on Supercomputers," by Crico

"Distillation Optimization," by Kumar and Lucia

Papers in Session II include:

"A Reduced Hessian Strategy for Sensitivity Analysis of Optimal Flowsheets," by Ganesh and Biegler

"Simultaneous Optimization and Heat Integration with Process Simulators," by Lang, Biegler, and Grossman

"An Improved Technique for Worst Case Identification," by Swaney and Kabatek

"Computer Simulation and Evaluation of Schemes for Detecting and Identifying Gross Errors in Process Data," by Rosenberg, May, and Iordache

"Scheduling in Multistage Serial Noncontinuous Processes with Finite Intermediate Storage," by Karimi

"Discrete Models for Gas-Solid Reacting Systems," by Sandman and Zygourakis

"On the Design of a Block-Diagram-Based Signal Processing and Simulation Package," by Preisig and Rippin

Papers in Session III include:

"Adaptive Local Thermodynamic Property Approximation in Process Simulation: Liquid Activity Coefficients," by Clark and Reklaitis

"Dynamic Simulation of Polypropylene Reactor Runaways for Safety Analysis of Relief Systems," by Kaushik and Augustine

"Stability of a Steady-State Hydrometallurgical Solvent Extraction Model," by O'Quinn, Frantz, and Van Brunt

"Dynamic Simulation of Complex, Multi-Stage Reactor Systems by a Modified DSS/2 Simulator," by Pirkle and Schiesser

"Parametric Sensitivity Analysis of Complex Process Flowsheets Using Sequential Modular Simulation," by Leis, Galligher, and Kramer

"Optimum Separation of Strongly Non-Ideal Fermentation Products: Steady State and Dynamic Simulation," by Wali and Karim

6.   **Synthesis.**   George Stephanopoulos   (Chairman), Department of Chemical Engineering, MIT, Cambridge, MA 02139, (617) 253-3904 and Rakesh Govind (Vice Chairman), Department of Chemical Engineering, 697 Rhodes Hall (ML 171), University of Cincinnati,

Cincinnati, Ohio 45221-0171, (513) 475-2761. Papers include:

"An Overall Strategy for the Systematic Synthesis and Optimization of Large-Scale Chemical Processing Systems," by Tedder

"Synthesis of Solids Processes," by Rossiter and Douglas

"An Algorithmic Method for Reactor Network Synthesis," by Achenie and Biegler

"Recent Advances in Reaction Path Synthesis: Computer-Assisted Prediction of Reaction By-Products," by Govind

"A Mathematical Modeling Approach to the Synthesis of Separation Sequences," by Lin and Prokopakis

"Multi-Effect Extractive Distillation for Separating Aqueous Azeotropes," by Lynn and Hanson

"Synthesis of Supercritical Extraction Processes," by Chimowitz, Kelley, and Munoz

"Synthesis   and   Design   of Heterogeneous Distillation Sequences," by Pham and Doherty

"Design of Molecules With Desired Properties,"   by   Joback   and Stephanopoulos

Joint Areas 10a and 10b Session

7-8.   **Perspectives in Computer-Aided Design and Operation. I. Steady-State Models for Design and Operation.   II.   Dynamic Modeling and Process Control.** John D. Perkins (Chairman), Department of Chemical Engineering, University of Sydney, Sydney, NSW 2006, Australia and Gerry R. Sullivan (Vice Chairman), Department of Chemical Engineering, University of Waterloo, Waterloo, Ontario N2L 3G1,

Canada, (519) 885-2196. Papers in Session I include:

"Analysis and Synthesis of Reactive Separation Systems," by Barbosa and Doherty

"Relaxation Strategy for the Structural Optimization of Process Flowsheets," by Kocis and Grossmann

"Heat Shunts and the Design of Energy Efficient Evaporator Systems," by Westerberg and Hillebrand

"The Artificial Intelligence Perspective in Computer-Aided Process Design," by Kriticos and Stephanopoulos

"Speedup: Recent Advances in Process Simulation," by Pantelides

Papers in Session II include:

"Observability and Redundancy Classification in Multicomponent Process Networks," by Kretsovali and Mah

"Multivariable   Time   Delay Approximations for Analysis and Control," by Holt and Galloway

"Adaptive Algorithms for Dynamic Simulation," by Cameron and Gani

"Robust Adaptive Controller Synthesis Methodology Based on the IMC Structure and the H-Two, H-Infinity, and Mu-Minus Optimal Control Theories," by Zafiriou and Morari

Area 10b Sessions

1.   **The Relative Gain Array–A 20 Year Retrospective.** V. Manousiouthankis (Co-Chairman), Department of Chemical Engineering, UCLA, Los Angeles, CA 90024, (213) 825-9385 and Thomas McAvoy, Department of Chemical Engineering, University of Maryland, College Park,

MD 20742, (301) 454-4593. Papers include:

"Relative Gain Analysis: A Historical Perspective," by Shinskey

"The Relative Gain Array for Units in Plants with Recycle," by Papadourakis, Doherty, and Douglas

"A Complete Interpretation of the Dynamic Relative Gain Array," by Slaby and Rinard

"Robust Performance of Decentralized Control Systems," by Grosdidier and Morari

"Progress in Synthesis of Decentralized Control Structures," by Manousiouthakis and McAvoy

"Nonlinear Loop Interaction," by Boe, Hwang, and Chang

2. Unsolved Problems in Process Control. Manfred Morari (Chairman), Department of Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, (818) 356-4186. Papers include:

"Articulating the Process Control Design Problem," Stephanopoulos, Johnson, and Lakshmanan

"The Dimensionality Problem of State Networks Used for Describing Sequentially Operating Plants," by Preisig and Rippin

"The Application of Automata and Formal Language Theory to Chemical Process Control," by Ydstie

"Practical Process Control of Distributed Parameter Systems–What are the Principles," by Ray and Gay

"Unsolved Problems and Needs of Process Control: A System Philosophy View," by Bristol

"Process Control: Research Goals for the Next Decade," by Morari, Economou, Zafiriou, and Doyle

3-4. Recent Advances in Process Control I and II. Karen McDonald (Co-Chairman), Department of Chemical Engineering, University of California, Davis, CA 95616, (916) 752-8314 and Joseph D. Wright (Co-Chairman), Xerox Research Centre of Canada, 2660 Speakman Drive, Mississauga, Ontario, Canada L5K 2L1, (416) 823-7091. Papers in Session I include:

"An Optimizing Control Scheme for Packed Bed Reactors," by Windes and Ray

"Adaptive Optimizing Control of a Semibatch Polymerization Reactor," by Houston and Schork

"Design and Control of Tubular Autothermal Reactors: An Evolutionary Approach," by Chylla, Adomaitis, and Cinar

"Performance Comparisons of Internal Model Control and Predictive Control," by Lee and Levien

"Dynamic Compensation for the Optimizer in a Large Process Unit," by Smith, Baxley, and O'Neill

"Selection Techniques for Process Model Based Controllers," by Cott, Reilly, and Sullivan

Papers in Session II include:

"Control of Ill-Conditioned Plants: High Purity Distillation," by Skogestad and Morari

"Forward Modelling Controllers: A Comprehensive SISO Controller," by Otto

"Design of Discrete Multivariable Linear-Quadratic Controllers Using

Transfer Functions," by Harris and MacGregor

"Multivariable Nonlinear Self-Tuning Controller," by Agarwal and Seborg

"Multivariable Adaptive Control With the Generalized Analytical Predictor," by Pavlechko, Edgar, and Wellons

"Bilinear Model Predictive Control," by Yeo and Williams

Joint Area 10b and Area 15 Sessions

5-6. Parameter Estimation and Process Control of Biochemical Engineering. M. Nazmul Karim (Chairman), Department of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO 80523, (303) 491-5252 and Ka-yiu San (Vice Chairman), Department of Chemical Engineering, Rice University, Houston, TX 77251, (713) 527-8750. Papers include:

"Estimation of the Growth Associated with Time-Lag Parameters in a Fermentor," by Wang and Stephanopoulos

"Nonlinear Adaptive Optimization of a Continuous Bio-Reactor," by Golden, Pangrle, and Ydstie

"Orthogonal Collocation Approximation for Parameter Identification and Optimal Control of a Distributed Parameter Biological Reactor," by Isaacs

"Dynamic Optimization of the Enzymatic Lysis of Yeast," Liu, Prokopakis, and Asenjo

"Utilization of Acid-Production Measurements for State Estimation and Control of Fermentors," by Koshy and Agrawal

"Algorithm for Adaptive Control of Activated Sludge Processes," by Papadoulis, Lyberatos, and Svoronos

"Adaptive Dissolved Oxygen Control and On-Line Estimation of Oxygen Transfer and Respiration Rates," by Holmberg and Olsson

"Extended Kalman Filtering with Physiological Modeling Applied to Baker's Yeast Fermentation," by Rajab, Pons, Dantigny, and Engasser

Area 10c Sessions

1-2. Impact of Advanced Computer Architectures in Chemical Engineering Computing I and II. Mark Stadtherr (Chairman), Department of Chemical Engineering, University of Illinois, Urbana, IL 61801, (217) 333-0275 and Michael A. Malachowski (Co-Chairman), Amoco Production Company, 4502 E. 41st Street, P.O. Box 3385, Tulsa, OK 74102. Papers in Session I include:

"Advanced Computer Architectures–An Overview," by Stadther, Coon, and Vegais

"Effective Utilization of Parallel Vector Processors," by Levesque

"Optimization of Algorithm Performance on a Cray-2," by Zygourakis and Markenscoff

"Waveform Relaxation Methods for Solution of Large Systems of Stiff Differential Equations," by McRae and Peckny

"Parallel Algorithms for Flowsheet Dynamics," by Carmola and Chimowitz

"Vector and Parallel Algorithms for Sparse Matrix Problems in Flowsheeting," by Vegeais and Stadtherr

Papers in Session II include:

"Supercomputer-Aided Analysis of 3-D Magnetohydrostatic Equilibria," by Boudouvis and Scriven

"A Computational Model of Productivity in Hollow-Fiber Bioreactors," by Decker, Hanson, and White

"Simulation of Complex Flows in Chemical Vapor Deposition Reactors," by Moffat, Kieda, McKenna, and Jensen

"Transfer-Matrix Method for Calculation of Transport and Mechanical Properties of Disordered Systems," by Sahimi

"Supercomputer-Aided Analysis of Transient Response of a Coating Operation," by Katagiri and Scriven

"Utilization of An Array Processor in Chemical Engineering Computations," by Cummings

"Simulation of Large Dynamic Systems," by Senior

3. Special Purpose Computers and Processing Systems. Peter R. Rony (Chairman), Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061, (703) 961-7658 and Daniel A. Crowl (Vice Chairman), Wayne State University, Detroit, MI 48202, (313) 577-3800. Papers include:

"A Computer-Aided Laboratory for Artificial Intelligence Applications in Chemical and Biochemical Engineering," by Stephanopoulos

"Tutorial: Digital Signal Processor (DSP) Integrated Circuits," by Galbo

"Chemical Network Problems Solved on NASA/Goddard's Massively Parallel Processor (MPP) Computer," by Carmichael, Cho, and Cohen

"An Integrated Hardware-Software Peripheral System for Dynamic Simulation," by Coulman

"A Computer Applications System for the Processing of Cave Survey Data," by Crowl

"Symbolic Computation and Chemical Engineering Model Development," by Sunol

Houston AIChE Meeting
(March 29-April 2, 1987)

Area 10a

1. Process Data Reconciliation and Rectification. Cameron M. Crowe (Chairman), Department of Chemical Engineering, McMaster University, Hamilton, Ontario, Canada L8S 4L7, (416) 525-9140 x-4947 and William Y. Svrcek (Vice Chairman), Department of Chemical Engineering, University of Calgary, Calgary, Alberta, Canada T2N 1N4, (403) 220-5755. Papers include

"Effect of Redundancy on Estimation Accuracy in Process Data Reconciliation," by Kretsovalis and Mah

"Detection and Reconciliation of Measurement Errors in Gas Distribution Systems," by Heenan, Cardiel, and Serth

"Interval Analysis as a Tool for Data Rectification," by Himmelblau

"A Hybrid Algorithm for Detection of Gross Errors in Linearly Constrained Data," by Serth, Johnston, and Heenan

2-4. Modern Applications of Chemical Engineering Theory I, II, and III. Richard Pollard (Co-Chairman), Department of Chemical Engineering, University of Houston, Houston, TX 77004, (713) 749-2414

and Mark E. Orazem (Co-Chairman), Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22901, (804) 924-6282. Papers in Session I include:

"Theoretical Analysis of a Rotating-Disk Chemical Vapor Deposition Reactor," by Coltrin, Breiland, Evans, and Kee

"Modeling and Analysis of Plasma Etching Reactors," by Economou and Alkire

"The Structure of DC Negative Glow Discharges," by Huffstater and Graves

"Temporal and Spatial Resolution of Optical Emission in RF Plasmas," by Jellum and Graves

"In-Situ Characterization of Surface States, With Application to Photoelectrochemical Semiconductor Processing," by Bonham and Orazem

"Modeling of Thermal Oxidation of Silicon," by Singh, Schlup, and Fan

Papers in Session II include:

"Stochastic Modeling and Control of a Semiconductor Etch Process," Rhinehart and Wu

"The Computer Simulation of Melting, Freezing, and the Glass Transition for Simple Materials," by Clancy and Chokappa

"A Mathematical Model for the Rate and Uniformity of Deposition in a Planar Source Diffusion System," by Yeckel and Middleman

"Fundamentals of Powder Production Using Aerosol Reactors," by Nguyen, Wu, and Flagen

"Mathematical Modeling of Coarsening in Phase-Separated Polymer/Solvent Systems," by Caneba

"Polypropylene Powder Compaction at Temperatures Above Tg," by Wang

Papers in Session III include:

"Reaction Sintering of Submicron Silicon to Produce Dense Si3N4 Ceramics," by Gregory and Lee

"Gas Phase Synthesis of Silicon Carbide Powders," by Mehosky

"Application of Chemical Engineering to Friction Materials (Composites)," by Shah

"Color Shifts of High-Solids Paints in Circulation Systems," by Service

"The Electronics Industry: Opportunities for Chemical Engineers," by Goldman

"Composite Airframe Structures: Can Thermoplastics Compete with Thermosets?," by Margolis

5. **Retrofitting and Optimization.** A. L. (Pete) Parker (Chairman), Shell Oil Co., P.O. Box, Norco, LA 70079, (504) 465-7459 and Edward Gordon (Vice Chairman), Fluor Engineering Inc., C4E, 3333 Michelson Drive, Irving, CA 92730, (714) 975-3531.

For further details, contact Jeffrey J. Siirola (Chairman, Area 10a), ECD Research Laboratories, Eastman Kodak Co., Kingsport, TN 37662, (615) 229-3069.

Joint Areas 10a and 11b Sessions

1-2. **Expert Systems and Computational Methods in Process Safety I and II.** V. Venkatasubramanian (Chairman), Department of Chemical Engineering, Columbia University, New York, NY 10027, (212) 280-4453 and Ernest J. Henley (Vice Chairman), Department of Chemical Engineering, University

of Houston, Houston, TX 77004, (713) 749-4407.

Area 10b

1. **Recent Advances in Computer Control.** Jorge Mandler (Chairman), Department of Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, (818) 356-4115.

2. **Distillation Tower Control.** John Slaby (Co-Chairman), Halcon and Karlene Hoo (Co-Chairwoman), Exxon Chemicals.

3. **Control of Chemical Reactors.** Herman Bozenhardt (Chairman), Fisher and Porter.

For further details, contact Thomas J. McAvoy (Chairman, Area 10b), Department of Chemical Engineering, University of Maryland, College Park, MD 20742, (301) 454-4593.

Area 10c Sessions

1-2. **Networking I and II.** Edward Gordon (Co-Chairman), Fluor Engineers, Inc., C4E, 3333 Michelson Drive, Irvine, CA 92730, (714) 975-3531 and Bill Alper (Co-Chairman).

3-4. **Human Factors and Computing Interfaces I and II.** Rajeev Gautam (Chairman), Union Carbide Corporation, P.O. Box 8361, South Charleston, WV 25303, (304) 747-3710 and Larry Biegler (Co-Chairman), Department of Chemical Engineering, Carnegie-Mellon University, Schenley Park, Pittsburgh, PA 15213, (412) 578-2232.

For further details, contact Norman E. Rawson (Chairman, Area 10c), IBM Corporation, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 564-5959.

1987 American Control Conference
(June 10-12, 1987)

The American Automatic Control Council will hold the 6th American Control Conference at the Hyatt Regency Hotel in Minneapolis, Minnesota. Two types of papers are being sought: those that describe work in some detail and shorter papers (approximately 700 words) that discuss recent results. Topics of interest include, but are not limited to: linear and nonlinear systems, identification and estimation, signal processing, multivariable systems, large scale systems, robotics, guidance and control, sensors, simulation, adaptive control, optimal control, and expert systems. Six copies of prospective papers should be sent to Yaman Arkun, School of Chemical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0250, (404) 894-2871 by September 15, 1986. Those who would like to organize sessions should contact M. Edward Womble, MS 6-14, Tracor Aerospace Austin, 6500 Tracor Lane, Austin, Texas 78725, (512) 929-2621 by September 15, 1986. (EDITOR'S NOTE: "Deadline . . . will probably pass by the time the newsletter is published, but it would be nice to let the people know about the program. A general call for papers appeared earlier in CEP.") The final selection of contributed and invited papers will be announced by February 1, 1987, at which time the authors' kits will be mailed. The General Chairman is Thomas F. Edgar, Department of Chemical Enginering, University of Texas, Austin, Texas 78712, (512) 471-3080. AIChE Invited Sessions under development include:

Nonlinear Process Control (Developers: J. Kantor, Notre Dame, and C. Kravaris, Michigan)

Expert Systems in Process Control (Developers: T. J. McAvoy, Maryland, and R. Moore, Lisp Machine)

Adaptive Control (Developers: W. K. Lee, Ohio State, and C. Tsiligiannis, City College of CUNY)

Recent Developments in Process Control (Developers: A. Palazoglu, UC Davis, and B. Holt, Seattle)

Applications of Advanced Process Control (Developers: K. Levien, Oregon State, and T. Taylor, 3M)

Robust Control for Processes with Constraints (Developers: E. Zafirou, Maryland, and M. Morari, Caltech)

Modeling and Control of Distributed Parameter Systems (Developers: J. B. Rawlings and B. W. Bequette, University of Texas at Austin)

Foundations of Computer-Aided Process Operations
(July 5-10, 1987)

H. Dennis Spriggs, Linnhoff March, P. O. Box 7577, Charleston WV 25356, (304) 776-1358 and Rex Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089.

Area 10c is planning this conference. Additional details are published elsewhere in this newsletter.

Minneapolis AIChE Meeting
(August 16-19, 1987)

No CAST sessions are planned.

New York City AIChE Meeting
(November 15-20, 1987)

Area 10a Sessions (Tentative)

1.   **Design and Analysis.** Richard S. H. Mah (Chairman), Department of Chemical Engineering, Northwestern University, Evanston, IL 60201, (312) 491-5357 and Iftekhar Karimi (Vice Chairman), Department of Chemical Engineering, Northwestern University, Evanston, IL 60201.

2.   **Applied Mathematics.** D. Ramkrishna (Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4066 and Christos G. Takoudis (Vice Chairman), School of Chemical Engineering, Purdue University, (317) 494-2257.

3.   **Complex Dynamics.** Michael F. Doherty (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413), 545-2359 and Julio M. Ottino (Vice Chairman), Department of Chemical Engineering, California Institute of Technology, Pasadena, CA 91125.

4.   **Computer-Aided Design of Batch Processes.** Kris R. Kaushik (Chairman), Shell Development Company, P.O. Box 1380, Houston, TX 77251, (713) 493-8525 and G. V. Reklaitis (Vice Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089. Topics of interest include: design synthesis and sizing; design under uncertainty; retrofitting applications; and plant layout studies. Deadline for the submission of preliminary abstracts is January 31, 1987.

5.   **Expert Systems.** H. Dennis Spriggs (Chairman), Linnhoff March, P.O. Box 7577, Charleston, WV 25356, (304) 776-1358 and V. Venkatasubramanian (Vice

Chairman), Department of Chemical Engineering, Columbia University, New York, NY 10027, (212) 280-4453.

For further details, contact Jeffrey J. Siirola (Chairman, Area 10a), ECD Research Laboratories, Eastman Kodak Co., Kingsport, TN 37662, (615) 229-3069.

Joint Areas 10a and 1b Sessions (Tentative)

1-2. **Bifurcation and Nonlinear Phenomena I and II**, R. Narayana (Co-Chairman), Department of Chemical Enginering, University of Florida, Gainesville, FL 32611 and G. Lyberatos (Co-Chairman), Department of Chemical Engineering, University of Florida, Gainesville, FL 32611.

Joint Areas 10a and 10b Session (Tentative)

1. **Integration of Process Design and Control**. Bradley R. Holt, Department of Chemical Engineering, BF-10, University of Washington, Seattle, WA 98195, (206) 543-0554 and W. David Smith (Vice Chairman), Polymer Products Department, E. I. DuPont de Nemours and Co., Wilmington, DE 19898.

Area 10b Sessions

1. **Batch Process Control**. Mark Juba (Chairman), Eastman Kodak Co., Bldg. 337, Kodak Park, Rochester, NY 14650, (716) 558-3637.

2. **Nonlinear Control**. Jim Rawlings (Chairman), Department of Chemical Engineering, University of Texas, Austin, TX 78712, (512) 471-5238 and Yaman Arkun (Co-Chairman), Department of Chemical Engineering, Georgia Tech, Atlanta, GA 30332, (404) 894-2871.

3. **Expert Systems Applied to Process Control**. Richard Weber

(Chairman), Exxon Chemicals, P.O. Box 100, Baytown, TX 77520, (713) 428-6385.

4. **Adaptive Control**. Won Kyoo Lee (Chairman), Department of Chemical Engineering, Ohio State University, Columbus, Ohio 43210, (614) 422-6591.

5-6. **Recent Developments in Process Control I and II**. Evanghelos Zafiriou (Chairman of Session I), Department of Chemical Engineering, University of Maryland, College Park, MD 20742, (301) 454-2431; Amhet Palazoglu (Chairman of Session II), Department of Chemical Engineering, University of California, Davis, CA 95616, (916) 752-8774; and Thomas F. Edgar (Co-Chairman of both sessions), Department of Chemical Engineering, University of Texas, Austin, TX 78712, (512) 471-3080.

For additional information, please contact Thomas J. McAvoy, Department of Chemical Engineering, University of Maryland, College Park, MD 20742, (301) 454-4593.

Area 10c Sessions

1-2. **Advances in Optimization I and II**. Larry Biegler (Co-Chairman) and Ignacio Grossman (Co-Chairman), Department of Chemical Engineering, Carnegie-Mellon University, Pittsburgh, PA 15213, (412) 578-2228.

3. **Scheduling and Planning of Operations I and II**. Moe Sood (Chairman), Mobil R and D Corporation, P.O. Box 1026, Princeton, NJ 08546, (609) 737-4960 and G. V. Reklaitis (Vice Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089. Topics of interest include: process planning models, scheduling algorithms, scheduling of batch operations (both multiproduct and multipurpose), use of simulation

to support scheduling, inventory planning models and methods, interface between scheduling and control, maintenance planning approaches and hierarchical production control systems. Deadline for submission of preliminary abstracts is January 31, 1987.

4. **Scheduling Batch Processes**. G. V. Reklaitis (Co-Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089 and Moe Sood (Co-Chairman), Mobil R and D Corporation, P. O. Box 1026, Princeton, NJ 08546.

5. **On-Line Fault Administration**. Mark A. Kramer (Chairman), Department of Chemical Engineering, MIT, Cambridge, MA 02139, (617) 253-6508.

For further details, contact Norman E. Rawson (Chairman, Area 10c), IBM Corporation, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 564-5959.

New Orleans AIChE Meeting
(March 1988)

Area 10a Sessions

Possible Topics: **Modeling of Systems in Non-Traditional Areas** (Polymers?), **Industrial Applications of Expert Systems** (Joint with Area 10c, 2 sessions), **Industrial Applications of Data Reconciliation**, and **Synthesis**.

For further details, contact Michael F. Doherty (Area Chairman-Elect), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2359.

Area 10c Sessions (Tentative)

1-2. **The Role of Computers in Safety and Reliability I and II**.

Richard S. H. Mah (Co-Chairman), Department of Chemical Engineering, Northwestern University, Evanston, IL 60201, (312) 491-5357 and Ernest Henley, Department of Chemical Engineering, University of Houston, Houston, TX 77004, (713) 749-4407.

3-4. **Computer - Aided Engineering**. Rajeev Gautam (Co-Chairman), Rajeev Gautam (Chairman), Union Carbide Corporation, P.O. Box 8361, South Charleston, WV 25303, (304) 747-3710 and Pete Parker (Co-Chairman).

Joint Areas 10a and 10c Sessions

5-6. **Industrial Applications of Expert Systems I and II**. Moe Sood (Co-Chairman), Mobil R and D Corporation, P.O. Box 1026, Princeton, NJ 08546, (609) 737-4960 and Kris Kaushik (Co-Chairman).

For further details, contact Norman E. Rawson (Chairman, Area 10c), IBM Corporation, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 564-5959.

University of Massachusetts, Amherst, MA 01003, (413) 545-2359.

Area 10c

Possible Topics: Advanced Computing Architectures (2 sessions), Computer Integrated Manufacturing for the Process Industry (2 sessions), Computing in Research and Development, Computer Support of Plant Operations (2 sessions), and New Technology.

For further details and suggestions for topics and chairmen, contact Norman E. Rawson (Chairman, Area 10c), IBM Corporation, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 564-5959.

Washington D.C. AIChE Meeting
(November 1988)

Area 10a

Possible Topics: **Artificial Intelligence in Design and Control; Applied Math or Linear Analysis; Nonlinear Analysis or Probability Theory; Design and Analysis** (2 sessions), **Applications of Advanced Computing Architectures in Design**, and **Statistical Methods in Engineering** (Process QC, nonlinear parameter estimation, experimental design techniques, etc.).

For further details, contact Michael F. Doherty (Area Chairman-Elect), Department of Chemical Engineering,

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
1987 AWARD NOMINATION FORM*

A.   BACKGROUND DATA

1.   Name of the Award _____ Today's Date _____

2.   Name of Nominee _____ Date of Birth _____

3.   Present Position (exact title)

_____

4.   Education:

Institution	Degree Received	Year Received	Field
_____	_____	_____	_____
_____	_____	_____	_____
_____	_____	_____	_____

5.   Positions Held:

Company or Institution	Position or Title	Dates
_____	_____	_____
_____	_____	_____
_____	_____	_____

6.   Academic and Professional Honors (include awards, memberships in honorary societies and fraternities, prizes) and date the honor was received.

7.   Technical and Professional Society Memberships and Offices

8.   Sponsor's Name and Address

_____
_____
_____

_____ Sponsor's Signature

_____

* A person may be nominated for only one award in a given year.

B.   CITATION

1. A brief statement, not to exceed 250 words, of why the candidate should receive this award. (Use separate sheet of paper.)

2. Proposed citation (not more than 25 carefully edited words that reflect specific accomplishments).

C. QUALIFICATIONS

Each award has a different set of qualifications. These are described in the awards brochure. After reading them, please fill in the following information on the nominee where appropriate. Use a separate sheet for each item if necessary.

1   Selected bibliography (include books, patents, and major papers published.)

2. Specific identification and evaluation of the accomplishments on which the nomination is based.

3. If the nominee has previously received any award from AIChE or one of its Divisions, an explicit statement of new accomplishments or work over and above those cited for the earlier award(s) must be included.

4. Other pertinent information.

D. SUPPORTING LETTERS AND DOCUMENTS

List of no more than five individuals whose letters are attached.

	Name	Affiliation
1.		
2.		
3.		
4.		
5.		

Please send the completed form and supplemental sheets by April 3, 1987 to the CAST Division Chairman, Dr. Thomas F. Edgar, Department of Chemical Engineering, University of Texas, Austin, TX 78712.