

Computing and Systems Technology Division Communications



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About This Issue

by Peter R. Rony and Joseph D. Wright

In this issue of CAST Communications, we publish a lengthy contribution, "The Future of Process Operations," from Prof. David Rippin. David is timing this article to start members of the CAST Division thinking about the forthcoming Foundations of Computer-Aided Process Operations (FOCAPO '93) conference in Crested Butte, CO (July 18-22, 1993). Further details about the conference will be published in the Summer 1992 and Winter 1993 issues.

CAST Communications finally has an official, AIChE-approved advertising policy. Professor Bruce Finlayson's ad for a new textbook is the first submission under this new policy, for which we have George Cominsky and his colleagues at CEP to thank. The important point is that the price structure for black-and-white ads is "based on the same cost per thousand (CPM) as Chemical Engineering Progress." In announcing these rates, the hope of AIChE is that potential advertisers of computer hardware and software would be willing to piggyback ads in CAST Communications with their ads in Chemical Engineering Progress (CEP). Bills for advertising in CAST Communications will be separately administered by the secretary/treasurer of the CAST Division; checks should be made payable to the CAST Division of the AIChE. Color advertisements would have a separate price structure, to be determined; inquiries are invited.

We request immediate attention by members of the Division to our Call for Recommendations for a 1993 CEP special issue on "Computing in Chemical Engineering." The CAST Division Executive Committee hopes to produce one of the most informative and effective issues of CEP ever published.

Call for Recommendations for a 1993 CEP Special Issue on "Computing in Chemical Engineering"

by Peter R. Rony and Joseph D. Wright

At the Los Angeles AIChE National Meeting in November 1991, the CAST Division Executive Committee invited Mark D. Rosenzweig, editor-in-chief of Chemical Engineering Progress (CEP), and Gary M. Rekestad, publisher of CEP, to consider potential CAST Division contributions to the publications activities of AIChE. As a consequence of such discussions, the CAST Division proposed to be responsible for a special issue on "computing" in CEP during 1993, to be published during the summer of fall of the year. According to CEP deadlines, the editors would require, by March or April 1992, an advance commitment to a firm table of contents for the 24 typeset pages of technical articles in the proposed issue.

Members of the CAST Executive Committee perceive this invitation as an opportunity to put the Division's "best foot forward" to the entire 50,000+ membership of the AIChE. We would like to produce a high-quality technical issue of broad interest and value to a majority of the AIChE members. Such an issue would provide a service to Society members, a consequence of the expertise in computing that members of the division possess. Further, an outstanding issue might serve to increase membership in the CAST Division, which has been stagnant at approximately 1800-2000 members for the past several years.

On behalf of the Executive Committee, the Publications Board hereby issues an invitation to all members of the CAST Division to immediately—repeat, immediately—convey their recommendations on the following aspects of the special issue:

- Specific theme of the special issue on "Computing in Chemical Engineering."
- Specific topics for technical articles that would have broad appeal to the AIChE members.
- Specific recommendations for authors of the technical articles, who would be given one year advance notice to provide them; self nominations would be accepted.
- Specific recommendations for an editor of the special issue, who would work in conjunction with the CAST Division publications board and the editors of CEP.

Observe that we have published this "Call for Recommendations" as the second item in the 1992 winter issue of the newsletter. This is a high priority request, and we encourage all interested Division members to give their immediate attention to it. Our objective is to make the theme issue a divisional response to the needs of the total AIChE membership.

Please respond immediately by mail or by E-mail to the editor of CAST Communications, Peter Rony.

To initiate your thinking on the special issue, the Publications Board has identified one possible theme, which we wish to share with you at this time. The flavor of our thinking can be summarized by the title, "Chemical Engineering Computing Using 100-MIPS Desktop Machines." The point is that very soon—only a matter of years—chemical engineering professionals will have 100-MIPS (where one MIP corresponds to one million instructions per second) computing capability on their desktops. We arrived at this title by asking ourselves, What will chemical engineers be doing with computing within several years? What would they do with a 100-MIPS machine on their desks? Of several possible answers—including more widespread supercomputing and sophisticated

computer visualization—we concluded that issues related to the 100-MIPS desktop machine had broader impact and might lead to a greater variety of technical articles. The theme issue would aim to be provocative. With 100-MIPS machines widely available, would the proverbial and frequently discussed “paradigm shift” in chemical engineering finally be at hand?

If we accept such a premise, what are the implications—for engineering management, engineering design, engineering operations, process controls, engineering research, engineering education, and so forth—of the widespread existence of such machines? We have assumed that the available RAM memory, hard disk memory, computer visualization graphics, communications rates, computer networking capability, and so forth would all be commensurate with machines with 100-MIPS capability.

Possible technical articles—none of which need to be lengthy—for the 1992 CEP special theme issue could include, but would not be limited to:

- 100-MIPS computer hardware: platforms, processors, parallel processors, architectures, memory, protocols, communications, graphics, multimedia, networking, cost, size, portability, etc.
- 100-MIPS computer software: size, speed, cost, operating systems, graphical user interfaces, visualization, databases, CAD, CAE, CASE, tools, networking, communications, training, education, operations, controls, research, materials, applications, and so forth.
- 100-MIPS molecular and engineering materials computing
- Managing the corporate 100-MIPS computing environment: the empowerment of engineering professionals

- Design opportunities with 100-MIPS machines
- Undergraduate and graduate education in the 100-MIPS academic computing environment
- Entrepreneurship/consulting and the 100-MIPS machine
- Real-time idea processing with the 100-MIPS machine
- Pharmaceutical R&D and the 100-MIPS machines
- ... and so forth

In the January 6, 1992 issue of *Electronic Design*, a high-performance CPU to be disclosed at the International Solid State Circuits Conference (ISSC) during February 19-21, 1992 is the following:

“...a 289-MFLOPS supercomputer on a chip developed by Fujitsu Ltd, Atsugi, Japan. Also fabricated in CMOS, the processor operates at 70 MHz and achieves a 289-MFLOPS throughput for single-precision computation and 149-MFLOPS for double-precision operations. To move data on and off the chip quickly, designers implemented a bus that can transfer 560 Mbytes/sec. To perform the computations, the processor contains six vector pipelines, four of which operate simultaneously with four-way bank-structured vector registers containing 8 kbytes each.”

In the January 28, 1992 issue of *PC Magazine*, it is reported that Bill Gates, chairman of Microsoft, predicts the following for PCs and software later in the nineties:

“Within three to five years, PCs using the Intel 80586 or Windows-compatible MIPS 4000 chip will have ten times the power of today’s SX-based systems, yet cost no more than today’s SX.”

“Standard equipment will include a 400 Mb hard disk, a cheap removable rewriteable optical disk (not a CD-ROM) of 400-plus megabytes, and a 2048 x 2048 pixel color display.”

“By decade’s end, there will be just two kinds of networks: 10 megabit-per-second wireless and 100 Mb/sec fiber-optic.”

“The higher, 10 times CPU power may give PCs enough horsepower to display full-motion video on-screen.”

“Other likely displays (all in color) will include a 6144 x 4096 pixel ‘whiteboard’ for workgroups, a 1280 x 1024 pixel laptop display, and a 640 x 480 pixel wallet computer display.”

As a reference point concerning the desired quality of the submitted articles to the CEP 1993 special issue, please consider the November 1991 issue of *IEEE Spectrum*, with its series of feature articles on “Software: Design, graphics, math packages, and more.” In the editor’s opinion, some of the finest general-reading, technical articles written in science and engineering appear in *IEEE Spectrum*, which has won numerous awards over the years for its outstanding special features. The CAST Division Executive Committee desires a high-quality, attention-grabbing special issue that challenges all members of the AIChE with our perception of computing opportunities.

In summary, the Publications Board of the CAST Division would welcome proposals to write articles for the CEP Special Issue on “Computing in Chemical Engineering,” scheduled for sometime during the second half of 1993. Please respond immediately to the editor of CAST Communications, Peter R. Rony, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061. Office phone: (703) 231-6631 (leave message with secretary); home phone: (703) 951-2805; Fax: (703) 231-5022; and E-mail: RONY@VTVM1.

CAST Division 1992 Chairman's Message

by Ignacio E. Grossmann



As we start 1992, we would like to acknowledge the work performed by the 1991 Executive Committee who was behind the organization of activities and services of the CAST Division last year.

Programming of sessions of the CAST Division remained very strong in 1991. Under the coordination of Jeff Sirola, the Programming Board Chairman, the Division had a total of 41 sessions: 10.5 in the Spring Meeting, 4.5 in the Summer Meeting, and 26 in the Fall Meeting. The Division also co-sponsored the PSE Meeting at Montebello and several sessions at the American Control Conference.

Under the joint efforts of Peter Rony, the Publications Board Chairman, and Joseph Wright, the Associate Editor, the CAST Newsletter appeared twice during the year with useful news and information. The organization of the banquet, awards, elections, and committee meetings of the CAST Division were also a success, particularly because of the efforts of Rex Reklaitis, (1991 Chairman), Mike Doherty (current 1st Vice-Chairman), Joe Wright (1991 Past Chairman), and Maria Burka (Secretary/Treasurer). We would also like to welcome the new elected officers for 1992: David Smith,

2nd Vice-Chairman and the Directors Gary Cera and Jim Davis.

A significant accomplishment in 1991 was a new Long Range Plan for the CAST Division whose development was coordinated by the Past Chairman, Rex Reklaitis. This plan, which is described in another article in this newsletter, involved the active participation of all the officers of the CAST Division. The plan has identified areas where improvements are required and has suggested specific action items that will be implemented over the next few years.

Areas that will receive special attention in 1992 are programming, membership, and finances. It is likely that in the future we will see significant decreases in the number of sessions at the Fall Meetings. Therefore, modified formats of sessions, increased participation at Spring and Summer Meetings, and other options will be examined. Improved mechanisms for submission of papers and extended abstracts that can facilitate the work by authors, session chairmen, and officers will be another area of priority. While the CAST Division is still one of the major divisions of AIChE, its membership has remained essentially constant since 1986 (it is currently close to 2000). We will seek how to increase membership, particularly by targeting graduate students and B.S. practicing engineers. The number of members of these two groups is currently low. We intend to work with universities and local sections of AIChE to reach these groups. Finally, although the financial situation of the Division is such that we can meet our current expenses, the undertaking of new projects and activities such as holding computer demonstrations at AIChE Meetings and making available a CAST membership directory will require additional funds. We intend to examine the current rates for membership and explore the possibility of sales of the CAST

Newsletter to non-members of AIChE and/or of the CAST Division.

We hope to accomplish in 1992 a number of the objectives set by the Long Range Plan. If you think you can help or wish to suggest ideas for improving the activities and services of the CAST Division, please let us know.

CAST Division 1991 Chairman's Message

by G. V. Reklaitis

Introduction

The mission of the CAST Division is to further the application of mathematical and computing principles in chemical engineering, particularly with respect to analysis, design, and control of processes and management systems. This mission is achieved by pursuing three principal activities: AIChE session programming and specialist meeting organization, publications, and awards and recognition. The programming and meetings activity is supported through active collaboration with other divisions in the Institute as well as collaboration with other professional organizations with interests in computing and systems technology. The publications activity occurs principally through the Division newsletter, CAST Communications. The awards activity centers on three annual Division awards, with funding provided by industrial sponsors.

1991 Executive Committee

The CAST Division organizes its activities following its By-Laws and performs its functions through the Division Executive Committee consisting of the following individuals:

Dr. Joseph Wright, Xerox Research Centre of Canada, Past Chairman

Prof. G. V. Rex Reklaitis, Purdue University, Chairman

Prof. Ignacio Grossmann, Carnegie-Mellon University, First Vice-Chairman

Prof. Michael Doherty, U. of Massachusetts, Second Vice-Chairman

Dr. Maria Burka, National Science Foundation, Secretary/Treasurer

Dr. Henry Chien, Monsanto Company, Third year Director

Mr. Arthur Parker, Shell Oil Company, Third year Director

Prof. Lorenz Biegler, Carnegie-Mellon University, Second year Director

Dr. Mohinder Sood, Mobil R&D Corp., Second year Director

Dr. James Deam, Monsanto Chemical Company, First year Director

Dr. Mark Juba, Eastman Kodak Company, First year Director

Dr. Jeffrey J. Sirola, Eastman Chemical Company, Programming Board Chairman

Dr. Kris Kaushik, Shell Oil Company, Area 10A Chairman

Prof. Christos Georgakis, Lehigh University, Area 10B Chairman

Prof. Mark Stadtherr, U. of Illinois, Area 10C Chairman

Prof. Jeffrey Kantor, Notre Dame University, Area 10D Chairman

Prof. Peter Rony, Virginia Polytechnic Institute, Publications Board Chairman

Prof. Thomas Edgar, University of Texas, Austin, Council Liaison

The Executive Committee meets twice annually, on Monday evenings at the Annual Meeting and, normally, on Tuesday evenings at the Spring National Meeting. The annual business meeting of the Division occurs at the banquet held on Tuesday evenings of the Annual AIChE Meeting.

Programming

The planning and organization of sessions, symposia, and conferences is the foremost activity of the Division. CAST programs at regular AIChE Meetings, organizes specialist conferences, and cosponsors several international meetings.

Regular Sessions: Programming of sessions at regular AIChE meetings occurs through four area committees: Systems and Process Design (10A), Systems and Process Control (10B), Computers in Operations and Information Processing (10C), and Applied Mathematics and Numerical Analysis (10D). Programming of timely and relevant sessions has been a hallmark of the Division. Planning is done at least two years in advance and considerable effort is expended by the Programming Board to insure that requested sessions are fully subscribed and completed.

At the Spring National AIChE meeting the CAST division sponsored 10.5 sessions, one jointly with 16B. At the Summer meeting CAST organized five sessions, two jointly with other areas. This was a special effort by the Division as CAST does not normally program in the Summer to avoid conflicts with specialty conferences in the process systems engineering area. At the Los Angeles Annual Meeting, CAST presented 26 sessions. One of these sessions was jointly sponsored with the Society of ChE, Japan as the first step of a longer term cooperation in the field of Computer Integrated Manufacturing.

Plans are well underway for the 1992 meetings. At this time 13 sessions are planned at the New Orleans meeting and only 20 have been granted by the MPC at the Miami meeting. This will represent a reduction of 20% over 1991.

Speciality Conferences: The Division was co-sponsor with CACHE of the very successful Chemical Process Control IV meeting held February 17-22 at South

Padre Island. CAST was also involved in the Fourth International Symposium on Process Systems Engineering held in Montebello, Quebec, August 5-9. This triennial meeting is cosponsored by the European Federation of Chemical Engineers, the Japanese Society of Chemical Engineers, and the Canadian and U.S. Institutes. Area 10B was actively involved in the 1991 Automatic Control Conference held in Boston on June 26-28.

The next Foundations of Computer Aided Plant Operations is now being planned for Summer 1993, with Area 10C as co-sponsor. Area 10B will again participate in the 1992 American Control Conference. The apparent slack in programming in Summer, 1992 will be amply filled by the IFAC sponsored DYCORN-92 Symposium (April, U. of Maryland) and the two European Working Party Meetings, ESCAPE-1 (May, Denmark) and ESCAPE-2 (September, France).

Publications

The Division newsletter, "CAST Communications," continues to appear semi-annually under the able leadership of Editor Peter Rony and Associate Editor Joe Wright. The newsletter is now the primary mechanism for distributing the Calls for Papers for future meetings. For instance, the Summer 1991 issue featured the final call for papers for the New Orleans sessions, the final call for the 1992 ACC meeting, and the first call for the Miami meeting. The newsletter also normally includes information from the Executive Committee, announcements of Division planning meetings, a conferences and workshops calendar, awards, summaries of conferences which have been held, and timely articles of general interest to the CAST community. It has become necessary reading for anyone involved in the development and application of computing systems in chemical engineering.

Awards

The Division is pleased to announce the 1991 winners of its three awards. Professor Rudolphe Motard of Washington University is the recipient of the Computing in Chemical Engineering Award, sponsored by Simulation Sciences, Inc. and Dow Chemical. Dr. Jeffrey Siirola, Eastman Chemical Company, has won the 1991 Computing Practice Award, sponsored by Pergamon Press, and Professor Michael Mavrovouniotis, University of Maryland, is the 1991 Ted Petersen Student Paper Award Winner. This award is sponsored by Chem Share Inc. and IBM. All three of the winners are outstanding contributors to the computing field and active members of CAST. Further details of the accomplishments of the awardees are given in the Summer 1991 issue of CAST Communications. The awards were presented at the Division Banquet in Los Angeles.

Long Range Plan

This year the Executive Committee undertook a long range planning exercise in order to chart the future activities of the Division. A working meeting was held at the Houston meeting to discuss initial drafts and ideas proposed by small subcommittees corresponding to the seven key activity areas of the Division: programming and meetings, publications, membership, international and intersociety relations, finances, outreach within AIChE, and awards. The plan was revised during the summer and will be presented for full discussion and adoption at the Los Angeles Meeting. Some of the preliminary action items which resulted from this planning activity were presented to the membership in the Summer issue of CAST Communications and were discussed at the Council of Division Officers meetings in Madison in June and Pittsburgh in August.

Initiatives which were acted upon at the November meeting of the Executive Committee include increase of Division dues, institution of a subscription to CAST Communications by non-members, and mechanisms for improving the quality of CAST sessions. On behalf of the division, First Vice Chair Ignacio Grossmann has also formulated a proposal to simplify the processing of abstracts and paper acceptance forms for contributions to AIChE sessions. This proposal is being presented for consideration by the Institute. The Division is further undertaking an initiative to establish formal liaisons with similar focus groups in other national/international chemical engineering professional organizations. Such liaison is important for coordinating the planning of conferences and symposia and the development of mutually beneficial joint activities.

Membership growth is a key issue for the long term, as CAST has maintained its membership at about 2000 for the last several years. Given that the majority of the AIChE membership is unaffiliated with any division, CAST certainly has the scope to grow over the next five years. Several specific action items are under discussion to help bring this about, including a focus on raising awareness of the Division's activities among students and local section members.

Summary

The Division continues to be an active and valuable contributor to the Institute. It is effective because of dedicated volunteers who have brought CAST programming and publications to be among the strongest in AIChE. The Division continues to be the source of outstanding leaders in AIChE at the National level and to lead in the introduction of new technologies in the business of the Institute. As computing and systems become even more central to the chemical processing industries, especially, as

the means of bringing about the computer integration of chemical manufacturing, the CAST Division will need to develop ways of expanding its scope to make its activities relevant not only to researchers and technology developers but also to the broader range of practicing engineers.

CAST Division Long Range Planning, Interim Report

The CAST Division has launched a comprehensive long range planning activity this Spring. A working meeting of the Executive Committee was held at the Houston Meeting to discuss initial drafts and ideas proposed by small subcommittees, corresponding to the seven key activity areas of the Division. The plan was revised during the summer and will be presented for full discussion and adoption at the Los Angeles Meeting. We anticipate publishing the final plan in the Division Newsletter after the Fall meeting so as to inform and involve the entire membership.

Division Mission

To further the application of mathematical and computing principles in chemical engineering, particularly with respect to analysis, design, and control of processes and management systems.

Specific Goals and Action Items

The activities of the Division can be described in terms of seven main categories: programming and meetings, publications, membership, international and intersociety relations, finances, outreach within AIChE, and awards. The following is a synopsis of goals and action items under consideration in each activity area of the Division.

Programming and Meetings

Goal: To provide preferred forums for the direct interchange of ideas related to the technical specialties of the Division, including systems and process design, systems and process control, computers in operations and information processing, and applied mathematics and numerical analysis.

Selected Action Items:

1. Take formal and proactive steps to seek our regular joint sponsorship with other programming groups.
2. Consider special programming for the Summer National Meetings as a means of reaching practicing engineers.
3. Pursue alternative session formats, such as hybrid poster sessions and block agendas. Facilitate sessions, tutorials, and speakers on computing for regional or local chapter meetings.
4. Sponsor a speciality conference under area 10d, Applied Mathematics and Numerical Analysis. Rotate this and the other three speciality conferences on a four year cycle.
5. Promote increased quality of sessions and presentations by initiating procedures for monitoring and maintaining historical records on the quality of speakers, sessions, and session chairs, on attendance, and on the degree to which regular deadlines are met.
6. Work with National to streamline session planning and organization, abstract submission, and meeting program development through use of E-mail, data-bases, and other computing aids.

Publications

Goal: To help CAST members keep abreast of Division activities, including programming, meetings, awards, Executive Committee actions, and new developments in computing technology.

Selected Action Items:

1. Seek commercial sponsorship that would allow the Newsletter to have a color cover and would reduce the dominance of the cost of newsletter on the Division budget.
2. Find sponsor for annual issue to be sent to graduating ChE students.
3. Convert newsletter operation to 100% electronic submission of text.
4. In conjunction with National, develop a financial package which encourages advertising in both the CAST newsletter as well as CEP.
5. Obtain a sponsor for the Division Membership Directory.
6. Explore joint sponsorship of an appropriate research journal which reflects CAST interest areas, such as Computers & Chemical Engineering.

Membership

Goal: To increase division membership at least 15% by 1996 (target 2250).

Selected Action Items:

1. Increase student membership by sending issue of newsletter and appropriate flyer to student chapters and design/control researchers.
2. Increase number of B.S. level members by focussing on local sections: send Newsletter and appropriate flyer.
3. Increase the number of international members: display newsletter and appropriate flyers

at international process systems meetings.

4. Develop a poster with the CAST logo which would be displayed in front of the podium of each CAST Division session.

International and Intersociety Relations

Goals: To achieve recognition as the leading professional chemical engineering organization with computing and systems focus. Establish active collaboration with other professional organizations with impact in furthering computing and systems developments.

Selected Action Items:

1. Appoint Division directors to serve as liaisons with a number of related organizations, including European Working Party on Computer Aided Process Engineering, Society of Chemical Engineers, Japan, and TIMS/ORSA
2. Coordinate advance, cross-organization planning of meetings in the systems and related technical areas to avoid conflicts and enhance overall participation.
3. Develop joint membership arrangements, including provision of membership in CAST for members of other ChE oriented organizations outside of the US.
4. Arrange regular exchange of newsletter, meeting, and other relevant information with other societies and organizations.
5. Develop regular, formalized mechanisms for CAST participation in joint-sponsorship and planning of PSE, CPC, and FOCAP style meetings.

Finances

Goal: To maintain financial stability and self-sufficiency of the Division.

Selected Action Items:

1. Maintain the Division dues at a level consistent with divisions of comparable membership size and scope of activities.
2. Adopt a subscription rate for the Division newsletter for non-members and develop billing arrangements with New York Office.
3. Develop arrangements with National so that the Division shares in revenues for symposium volumes and other special publications initiated through Division initiatives.
4. Seek endowments for the three Divisional Awards to replace existing recurring funding.

Outreach within AIChE

Goal: To expand the awareness of the Division and its activities among other segments of the Institute.

Selected Action Items:

1. Champion the wider acceptance and utilization of computer technologies in AIChE activities such as New York office operations, programming activities, meeting arrangements, and publications.
2. Join with other divisions and programming groups (e.g., Fundamentals) in programming in Summer and Spring meetings.
3. Become proactively involved in recruiting and encouraging selected Division members to join the Speakers Bureau.
4. Work with larger local sections to organize one day symposia on new computing developments. Assist in the identification of keynote and

session speakers and assemble papers for distribution.

Awards

Goals: Recognize major technical and organizational contributions in chemical engineering related computing and systems technologies.

Selected Action Items:

1. Increase the level of the cash awards associated with the three CAST Division awards to levels in line with awards in other divisions: Computing in Chemical Engineering to \$2500, Computing Practice to \$2000, and Ted Peterson Student Paper Award to \$750.
2. Develop mechanisms for recognition of lower level achievements such as best paper awards given by theme or area at a regular AIChE meeting or speciality conference.
3. Seek funds to permanently endow the existing awards.

New CAST Division Officers

The new CAST division officers, elected late in 1991, are W. David Smith, 2nd Vice Chairman; Gary D. Cera, Director, 1992-94; and James F. Davis, Director, 1992-94.

W. David Smith
2nd Vice Chairman



When not skiing, Dave Smith is a Senior Supervisor at DuPont Polymers, where he has responsibility for most of the process modeling and advanced process control in that Sector. He leads a group of predominantly Ph.D. chemical engineers who focus on improving existing processes. In addition, he leads the New Technology Team of the Corporate Process Measurement and Control Center in the Engineering Function. This group has the responsibility to identify, evaluate, and introduce new process control technology into DuPont. Before working at DuPont, Dave taught at the University of Rochester for twenty years, where his main interests were chemical reaction engineering, process design, and applications of digital computers to chemical engineering. While in Rochester, Dave was active in the local section of the AIChE and, at one time or another, held every office in that organization. He earned his B.S. from Princeton and both M.S. and D.Eng. from Yale. The transition from

Yale to Rochester involved a very exciting detour to Australia on a Fulbright to study applied mathematics and computers in the Basser Computing Centre at the University of Sydney.

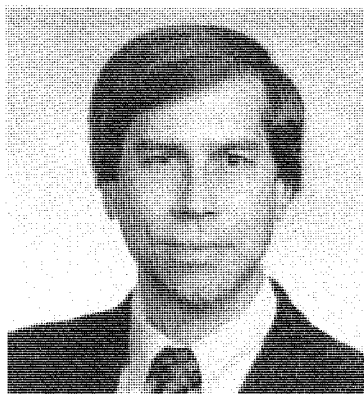
Gary D. Cera
Director, 1992-94



Gary Cera oversees the Computer-Aided Operations Group in the Process Engineering Division of Mobil's Corporate Engineering Department. He directs a group of individuals who are responsible for the development and deployment of advanced computing technology for process and economic improvement in Mobil's refining operations throughout the world. Recent projects in which he has been involved include advanced monitoring, simulation and optimization, and online advisory systems for reforming and catalytic cracking processes. Prior to joining Mobil Research and Development Corporation, he was a Research Engineer with E. I. du Pont de Nemours & Co. where he had technical assignments in process design and troubleshooting in the Petrochemicals Department, sensor research and development in the Polymers Department, and research into parallel computing for dynamic process simulation in the Central Research Department. Prior to his employment by Dupont, he was a Research Engineer with AMOCO Corporation, where he was responsible for the

automated collection and analysis of pilot plant data for material and energy balances for a large number of pilot plant and semiworks scale units ranging in complexity from alkylation to catalytic cracking. He holds a B.S. degree in Chemical Engineering from the University of Wisconsin and M.S. and Ph.D. degrees from the University of Illinois. His publications are primarily in the areas of electrochemical reactor and flowsheet modeling, optimization, and parallel computing. He regularly chairs sessions at AIChE conferences and he currently holds the position of Vice-Chairman of the CAST Division Area 10C. With an interest in computing in chemical engineering education, he is Mobil's industrial representative to the CACHE Corporation.

James F. Davis
Director, 1992-94



Jim Davis is an associate professor of Chemical Engineering at the Ohio State University (B.S. from U. Illinois; M.S., Ph.D. from Northwestern University). In addition to an academic background, he has an industrial process operations and control background with Amoco Chemicals Corporation and Argonne National Laboratory. For the past eight years, Jim's research work has been in the application of Artificial Intelligence (AI) to problems in the petroleum, chemical, and paper industries. Primary emphasis has been on the integration of knowledge-based

system and neural network technologies with conventional numeric approaches. This work has led to the implementation of knowledge-based systems to solve a variety of industrial problems. In addition, he has consulted for a number of companies on the application of these technologies. At Ohio State, he directs the AI in Chemical Engineering Group within the Laboratory for Artificial Intelligence Research and he currently teaches a course on the application of knowledge-based systems to engineering problems. He has presented numerous papers and has taught a number of short courses to both industrial and academic audiences. Jim is active in CACHE as an academic trustee and serves on the AI Task Force. Within AIChE he has been active in chairing and/or co-chairing technical sessions.

Advertising Rates for CAST Communications

by George Cominsky

Given below is a suggested price schedule for CAST Communications. It is based on the same cost per thousand as Chemical Engineering Progress (CEP):

1/4 page	\$ 60
1/3 page	\$ 70
1/2 page	\$ 90
2/3 page	\$120
1 page	\$150

I do not suggest using smaller sizes, such as 1/6 page. Payment for all ads should be by check payable to the Secretary/Treasurer, CAST Division, AIChE.

Articles

The Future of Process Operations

by D. W. T. Rippin, *Technisch-Chemisches Laboratorium, E.T.H. Zürich, CH-8092 Zürich, Switzerland*

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This informal contribution was presented at the workshop, "Computer Aided Process Engineering," organized by the Working Party of the European Federation of Chemical Engineering on Computer Aided Process Engineering at the World Congress of Chemical Engineering, Karlsruhe, Germany, June 1991. It also serves to set the scene for the Second International Conference on Foundations of Computer Aided Process Operations, FOCAPO-2, sponsored by the AIChE CAST Division and CACHE, to be held in Crested Butte, Colorado, July 1993. The joint chairmen of that conference, David Rippin (address above) and John Hale, Du Pont Engineering, P.O. Box 6090, Newark, DE 19714-6090, welcome comments and suggestions on this theme.

No attempt is made to give a comprehensive survey of the field of operations. The intention is to view the field as a whole and stimulate interest in its structure.

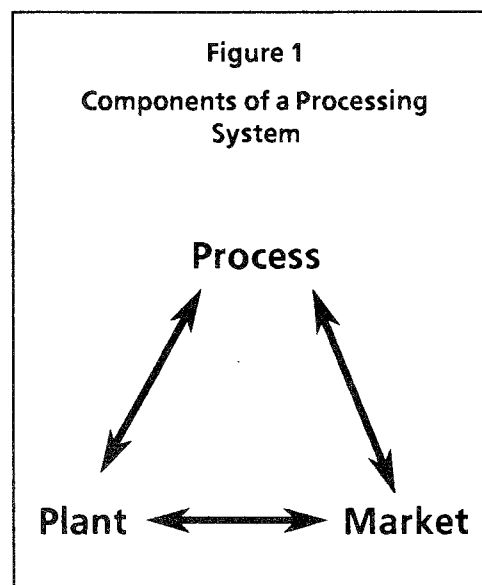
I want to say:

- why a discipline of process operations is needed
- what some of the components will be

and then to raise some questions about the place of process operations in teaching and research, and the role of chemical engineers compared with that of other disciplines.

Design is often described as the keystone of chemical engineering education. It is certainly of value for students to draw together what they have learned in an open-ended project requiring some initiative and originality. However, how many of them will have an opportunity to exercise this in practice? For many chemical engineers going into employment, it may be the keystone for an arch that is never constructed.

It has been suggested that few new "world size" plants will be constructed, at least in Europe in the coming years. The existing ones will be subject to increasing competition so that more attention will have to be paid to efficient operation. New plants are likely to be smaller and more flexible, needing to be continually matched to the marketplace in product quality and variety. All the operating manager's resources will be deployed to realize this matching in the most effective way, and he must be **equipped** (hardware, software, information) to make this matching effectively.



The change in emphasis in recent years can be illustrated by considering three necessary components of a processing system:

- Markets for one or more products.

- Process specifications—definition of the sequence of transformations or tasks which have to be performed to convert raw materials into products.
- A plant or set of equipment items in which the tasks can be performed.

These components must be interconnected in an appropriate manner. For a large continuous plant, *all three components are clearly defined.*

- A continuous plant will be built only if there is confidence that the *market* for the product will continue for a considerable number of years.
- All the tasks required to carry out the *process* must be well understood, so that a balanced plant can be designed; each task must accept material from upstream, process it, and pass it on downstream at the same rate.
- The tasks are assigned once and for all to the *plant* equipment items, usually specially designed for the purpose.

The *interconnections between the components are rigid*. The same product will be made by the *same* process in the *same* equipment through interconnections that are *fixed* at the design stage. Operators of large continuous plants hardly have to think about these interconnections, because they never change.

However, many products and groups of products in demand today do not have these characteristics. The processing components are not clearly defined:

- they are "fuzzy"

As a result the interconnections between the components are not rigid:

- they are **flexible**; they may even be continually changing.

Products are made in smaller, more flexible continuous plants or in batch plants.

- *markets* are not stable, may not be large and new products may be anticipated.
- *process* knowledge may well be limited, certainly insufficient to design a well balanced continuous plant.
- *process* operation may only be known in batch form, corresponding to laboratory procedures with no obvious transformation to continuous mode.
- *plant* equipment cannot be specially designed, it must be versatile, capable of handling different amounts of material and perhaps also different products.

Because the components are fuzzy, the interconnections must be flexible. *Different* products will be made, *different* processes will be used, process tasks will be realized in *different* equipment items at *different* times. The business and the technology are continually interacting.

For plants to be successful in a volatile, increasingly competitive environment, excellent design will certainly be required, but excellent design by itself will not be sufficient.

In the the plenary address which Roger Benson of I.C.I. gave to the process systems engineering conference PSE '88 in Sydney, Australia, he illustrated the improvements in design which could be achieved over a twenty year period in a small partial oxidation process—which is none other than the private car that most of us drive every day.

To emphasize the range of skills needed and choices available in process operations, I would like to carry the analogy between the car and the industrial chemical plant a little further. When a new car of the most advanced design is delivered to your doorstep, much additional information and many additional skills are needed

Figure 2 What is Needed to Operate a Well Designed Car?

Destinations or other objectives

Road maps

Owner's manual

Quality and availability of raw materials

Current state of plant

Anticipating and monitoring change

Auxiliary safety devices

Redundant equipment

Waste monitoring and treatment

Rules of the road

How other operators behave

to operate it successfully and get the maximum satisfaction from it.

You will have some desirable destinations in mind, or perhaps other objectives such as driving around to enjoy the sunshine (or impressing your partner with overtaking ability on the German Autobahn). You will need road maps to identify routes and the owner's manual to advise on starting and using the equipment and to give some elementary maintenance procedures.

Quality and availability of raw materials needs to be ensured. Will lead-free gasoline always be available? How can I monitor the current state of the plant during operation? (Speed; fuel level in the tank; some things are no longer revealed these days, like the charging rate of the battery; new

things appear, like the average fuel consumption). What maintenance procedures will be required for routine or emergency situations, and how can I be sure they will be available? How can I anticipate and monitor change in the state of the system and the environment and take necessary corrective action?

- the driver looks around and responds to what he sees ahead on the road.
- change in the condition of the car may be noted from the instrument readings, from warning devices, or from direct observation such as a change in the sound of the engine or the bump, bump of a flat tire.

Although the design of this plant should be intrinsically safe, there will be auxiliary safety procedures which must be used—"fasten your seat belts" (adjust your air bag?).

Some redundant equipment will be installed to improve overall reliability; some will be obvious, other redundancy will be hidden. I think we all still carry a spare wheel. How many still have spare bulbs, fuses, or a fan belt?

In Switzerland, waste is monitored by an obligatory annual emission control and all new plants have to have a waste treatment facility in the form of a catalytic after burner. We cannot drive unless we know the rules of the road, and how the other operators are going to behave. (I have not pondered what the industrial plant equivalent is of policemen and speed limits).

This analogy is intended to give an impression, from an abnormal perspective, of the range and diversity of factors that must be handled in an operating situation. We now consider more explicitly how these or similar factors arise in an industrial environment.

A large number of themes, in fact an *enormous* number of themes, impinge

on process operations. However, there is no recognized discipline within which all these themes can be fitted together so that we can recognize what considerations are relevant in what circumstances.

I would like to look at some simple questions, in the context of process operations, and see what a diverse range of factors may impinge upon them. First I consider how to characterize the operating situation and then how the plant and its ancillary facilities can be designed and operated to respond to this situation.

Figure 3
Identifying the Situation

Where are we going?

How do we know where we are?

What is changing?

What is going wrong?

Where Are We Going?

How are objectives formulated for production operations at different levels, from the plant to the works to the business? How are these conditioned by the nature of the production environment? For example, a commodity chemical may be required at a fixed rate and a given quality, or a batch production facility may be assessed by the service level of a range of products in a fluctuating market. How can the production environment in which the plant operates be characterized (what sort of a road map do we have of the competitive commercial surroundings in which the plant must operate)?

To what extent can technical and commercial factors be separated from

one another? Must process operations always be oriented to both?

How Do We Know Where We Are?

To judge the performance of a plant or to change the performance of a plant we need to know where we are—what is the current state of the plant. The plant people or the plant computer can observe instrument readings—the measurements may be insufficient or unreliable, in which case they must be improved.

In other cases *more* than enough information may be available, but it is inconsistent. If all the inputs and all the outputs of a unit are measured, the results may not be consistent with the mass or heat balances because of (a) inaccurate measurements, (b) unnoticed leaks, or (c) other reasons.

A sub-discipline has grown up of data reconciliation, which uses statistical methods to make the best estimate of system state on the basis of initially inconsistent data. *How much information* do we need to adequately define the state of a non-stationary system, a batch plant, a multipurpose plant? Is it just enough to estimate the current performance/objective function?

If by the state of the system we mean sufficient knowledge to predict how it will evolve in the future we may need much more detailed information:

- how much has the catalyst activity deteriorated?
- how much fouling is there in the heat exchangers?

such information may be deduced from records of recent behavior.

Alternatively, it may be possible to extract relevant information of similar circumstances in the past from archives of plant records which some companies have built up over many years of data recording. It seems that

exploitation of these data *mines* of process history has hardly begun.

How much data do we need? Where do we get it from? How do we massage it to know with sufficient confidence where we are and what state we are in?

What Is Changing?

As in the motor car, we try to look ahead to anticipate change. There are various methods of forecasting:

- extrapolation, time series, probabilistic estimates, scenarios.

What Is Going Wrong?

At the simplest level, something is noticed on the plant (like the flat tire on the car). At the next level a warning light flashes a computer message, for example, (a) some variable is out of control limits, or (b) some undesirable combination of events has been detected.

Sometimes disturbances are masked by noisy signals or infrequent measurements and can be exposed by methods of *statistical quality control* for detecting changes, for example, Shewhart control charts or cumulative sum charts. *Acceptance sampling* procedures can be used to check conformity to required standards. Of course all these procedures can be used to check not only product quality but also safety, environmental or other parameters.

Generally speaking, these methods detect only the symptoms. The process operator wants to know the causes of change. An experienced operator, on the basis of a *mental model*, may be able to suggest the likely causes for a certain combination of symptoms, or he may be able to suggest further observations or investigations.

Attempts are being made to reproduce or improve on this capability

Computer-assisted fault finding may use models of various kinds:

- a conventional mechanistic model to simulate the consequences of various faults.
- a qualitative model which retains some qualitative physical relationships, but makes only qualitative prediction.
- an expert system containing qualitative rules that seek to mimic the procedures of an experienced operator.
- a flexible empirical model that seeks to match patterns of events (perhaps under the name of a neural network).

Is Something Going Wrong?

- How do we recognize the symptoms?
- What models do we use to track down and correct the causes?

Of course, some error correction is built into the control structure of the plant. Errors are recognized and corrected by feedback mechanisms chosen in the control system design. These feedback mechanisms may range from simple linear controllers to complex models adapting to the changing situation.

Figure 4

Responding to the situation

Design to operate in a changing environment

Ancillary facilities to cope with change

Planning and realization of operational sequences

Planning to meet product demands

Planning to follow the market

Design to Operate in a Changing Environment

A plant operating in a changing and uncertain environment may be called upon to face different technical conditions and different market conditions. It will surely not be appropriate to design such a plant to a single reference performance at minimum cost. (I remember a senior I.C.I. engineer at a symposium entitled "Dropping the pilot" more than 20 years ago—when optimization was just becoming fashionable—saying something like: "When we built a plant in the old days, we knew conditions would always change after the plant was built, so we put in a bottleneck here and a bottleneck there, so that when conditions did change the bottlenecks could be relieved one after another, gradually modifying the performance without too much expense. These new 'optimized' plants are no use at all; they bottleneck all over the place, all at the same time and you cannot do a thing with them.")

A *really* optimal plant ought to have been built in an economically appropriate amount of flexibility taking account of the *value* of the flexibility in the anticipated environment, and the *cost* of providing it.

However, what should be done if the commercial environment is *very* unstable?

In some batch environments product mix may change, new products may emerge, plants may even be built without knowing what products will be produced in them. It will then be impossible to quantify the benefits of flexibility for the specific situation and other principles of design will have to be used, perhaps relying on experience of what types of equipment mix have been successful in the past in a similar environment. Experience associated with flexible manufacturing systems

(FMS) in the mechanical industries may offer some guidance here.

Flexibility should not be judged only on what the bare plant can do. What has to perform is:

plant

plant + control system

plant + control system + ancillary devices (storage to smooth out demand fluctuations or redundant equipment to smooth over unreliability)

plant + control system + ancillary devices + planning and scheduling procedures

plant + control system + ancillary devices + planning and scheduling procedures + business line management

How successful is the whole structure in operating in a complex, changing environment, and what is the appropriate contribution of each element?

Ancillary Facilities to Cope With Change

External to the actual plant, provision can be made to cope more effectively with change. Raw material and product stocks help to insulate the plant from external disturbances and intermediate stocks may alleviate the effect of breakdown of individual equipment items. Optimal stock levels can be determined by a trade-off between costs and benefits. However, generous stock levels may have been used in the past to give managers a quiet life.

On a larger canvas, more rapid communication of requirements from customer demand along the production and distribution chain ("just in time") can result in enormous savings in inventory cost. Change in status or capability of the plant calls for monitoring of reliability and devising of procedures for routine and

opportunity maintenance. Spare equipment items may also be installed to improve overall availability. Analytical mathematical procedures for simple cases and stochastic simulation for more complex ones are available for studying these situations.

Planning and Realization of Operational Sequences

Sequences of actions need to be planned for start-up, shut-down, product change-over, safety or emergency actions. Robots and experiences of CIM in other industries may be called upon here. Network or critical path planning or more recent developments such as Petri-nets may be relevant. Appropriate interfacing with humans involved in the sequence will also be important.

Planning to Meet Product Demands

Allocation of production resources and detailed scheduling of their use in time provide very challenging problems. Many practical problems are far too large for purely numerical computation. This is likely to be supplemented by heuristic or knowledge-based methods or interactive methods where the user also contributes to the plan.

Planning to Follow the Market

This implies still greater freedom than producing to a set of orders:

- "Just in time" production, plant wide control, coupling manufacturing to business.
- Integration of production with raw materials supply, distribution and customer service, general problems of logistics, materials flow ... etc.

And What About the Competition?

The ability to analyze and characterize the operating situation and to respond to it are conditioned by available *tools* and the ease with which they can be applied. Many tools and procedures are in routine use. Others are not sufficiently well known or user-friendly. The desirability of other tools has been recognized, but they are not sufficiently developed. Still other tools which will be widely used in the future have not even been recognized.

Some of the currently available tools can be classified as:

- *deterministic tools* for steady state and dynamic simulation optimization.
- *stochastic tools*: statistical methods, discrete event/stochastic simulation, and perhaps stochastic optimization.
- *knowledge-based tools* dealing with qualitative information.

I have presented operating problems in a series of levels, from the individual plant to approaching the corporate level. This is only one perspective. Operations can be viewed in many different dimensions under alternative classifications such as resources, requirements, and techniques.

Considerations of *safety, environment* and *health* will be all-pervasive as will be the need to *involve and motivate the people* concerned.

How to Fit Into a Consistent Discipline of Operations

A discipline of process operations is needed, not to give a rigid procedure through which every case has to pass. The number of possibilities is far too vast for that. However, a framework could help (a) *to characterize the nature of a process* in terms of the operational problems it will present, (b) *to characterize the operating environment* in which it must function, and (c) to put

these together *to identify bottlenecks/opportunities*.

For Further Discussion

1. Increasing pace and volatility of business call for increased attention to *operations* and computing or other tools to make them more effective. I have the impression that many chemical engineers emerging from university courses have little education in or even knowledge of operational problems and practices.
2. Does closer integration of market considerations with technical decisions mean that chemical engineers will be squeezed out of responsible decision making roles by business experts, or will ChEs be able to educate themselves, or be educated for a broader decision making role? (Might we have a specialization for an operations engineer over/against a design engineer?)
3. Is it appropriate for academics to be involved in research contributions to the *overall* field of operations and its structure, rather than expending their energies on little corners of the subject? How do they get access to relevant experience to form an overall view? Can the intellectual challenge and academic content of such work be more precisely formulated and more widely recognized?

I would like to acknowledge the discussions I have had on this subject with a number of colleagues from industry as well as university in Europe and the United States.

Communications

Chemical Engineering Optimization Models with GAMS

by Ignacio E. Grossmann, Carnegie Mellon University

CACHE has recently produced a new design case study, Vol. 6, "Chemical Engineering Optimization Models with GAMS." The objective of this case study is to provide a set of chemical engineering problems to supplement optimization courses at both the undergraduate and graduate level. This case study should also be of interest to practicing engineers who want to learn about GAMS and its applications.

Chemical engineering is a fertile area for optimization since many problems in our field can be modelled as problems in which an objective function is to be minimized or maximized subject to a set of equality and/or inequality constraints. While optimization is a conceptually powerful framework, its impact has been somewhat limited due to the lack of tools that facilitate the formulation and solution of these problems. For this reason in the past the teaching of optimization has been regarded mainly as an interesting theoretical exercise, but with limited applicability, except perhaps for the case of linear programming problems, which only constitute one type of optimization problems in chemical engineering.

Recent years, however, have seen the development of not only new algorithms, but also of powerful modelling systems. For instance, the advent of modelling systems such as GAMS has opened new possibilities for solving a great variety of optimization problems. The important feature of

modelling system like GAMS is that they provide an environment where the user need not be concerned with the details of providing the interfaces with various optimization codes (e.g. calling the appropriate routines, supplying the correct arguments for variables and functions with their derivatives, etc.). Instead, this environment automates the interfaces which allows the user to concentrate on the modelling of problems, which ultimately is the main skill that is required for the successful application of optimization in practice. More importantly, an environment such as GAMS greatly reduces the time—up to one order of magnitude—for the user to formulate and solve an optimization problem. It should be noted that other modelling systems that are available in chemical engineering are ASCEND from Carnegie Mellon and SPEED-UP from Imperial College. Both systems have capabilities for nonlinear optimization.

It is clear that a tool such as GAMS can have a profound impact in education and practice. It is for this reason that we have been motivated at CACHE to produce this case study to show how, with a tool such as this, one can cover in a course a large variety of optimization problems that are of relevance to chemical engineering. For educational reasons most of the problems in this case study are somewhat small in terms of size in order to be able to run them in PCs in reasonable times.

This case study covers applications at various levels of complexity in the following areas:

- Planning and scheduling of batch and continuous processes
- Chemical and phase equilibrium
- Design of heat exchanger networks, distillation columns and batch processes
- Synthesis of reaction paths, heat

exchanger networks and distillation sequences

- Optimization of dynamic and distributed parameter models

The above problems give rise to mathematical programming problems of the following type:

- (a) Linear programming (LP) which involves continuous variables and linear objective function and constraints.
- (b) Nonlinear programming (NLP) which involves continuous variables and nonlinear objective function and/or constraints.
- (c) Mixed-integer linear programming (MILP) which involves discrete (mainly 0-1) and continuous variables and linear objective function and constraints.
- (d) Mixed-integer nonlinear programming (MINLP) which involves discrete (mainly 0-1) and continuous variables and nonlinear objective function and/or constraints constraints.

This case study describes in some detail the formulation and solution of a total of 21 optimization problems that cover the 4 classes of optimization problems cited above. GAMS input files which are extensively documented, are provided for each of these problems. Some of these input files are rather general, almost like self contained programs where problems can be specified with different data and dimensionality.

The case study is organized as follows. First a brief tutorial introduction to GAMS is given to illustrate at the simplest level some of its capabilities, and how to use the program. Also, some useful hints are included in this section. Readers not familiar with GAMS should first read this section. For more details, the reader is referred to the GAMS User's Manual, which is provided with the case study. Next, the 21 problems are presented,

emphasizing the formulation of the problem, and discussion of results for which the input file of GAMS is also given (output listing files have been omitted except for the first problem due to space limitations). The GAMS input files of these problems are included in the diskette provided for the case study. For several of these files it is recommended that a 386 or 486 machine be used due to the time required to solve the problems. A number of suggested exercises have also been included in the description of each problem. At the simplest level they involve solving the same problem for different data, and at the more complex level they involve modifying the formulations or explaining certain features in the model or algorithm.

Finally, several appendices have been included. The first one is a guide for the use of the MINLP optimization code DICOPT++, which is a non-standard option in the commercial version of GAMS. This illustrates the fact that GAMS can also be used as an interface to special purpose algorithms. The second appendix shows how GAMS can be used to program an algorithm such as Generalized Benders Decomposition. Finally, an appendix is given to provide some background on how to convert optimization problems with differential equations into nonlinear programming problems.

This case study, which can be ordered from CACHE (see address below), includes the following items:

- (a) Special student version of GAMS for IBM-PC and compatibles (1 Megabyte memory recommended) in 3½" diskettes. The BDMLP, MINOS, ZOOM, and DICOPT++ codes are included in GAMS. Problems with a maximum of 1000 nonzero elements (300 nonlinear) can be solved.
- (b) GAMS input files for all the problems; these are extensively documented.

(c) GAMS User's Guide.

This case study has been prepared by faculty and students at Carnegie Mellon University (Larry Biegler, Ignacio Grossmann), Northwestern University (Iftexhar Karimi) and Princeton University (Chris Floudas). GAMS Development Corporation, the Licensing Technology Office at Stanford University, XMP Optimization Software and the Engineering Design Research Center at Carnegie Mellon have donated the computer software for this case study.

The price of case study is \$80 (\$55 for academics whose departments are CACHE members), and it can be ordered from CACHE Corporation, P.O. Box 7939, Austin, TX 78713-7939; Tel: (512) 471-4933. Please make the check payable to CACHE Corporation.

Highly Successful Software Demonstrations to Repeat in Miami

by Douglas J. Cooper

The AIChE 1991 Annual Meeting in Los Angeles this past November saw the introduction of the first "Demonstrations of Software for Chemical Engineering Education." The demonstrations, the brainchild of Professor Alan Foss of the University of California at Berkeley, showcased software developed by academics for use in chemical engineering instruction. Professor Douglas Cooper of the University of Connecticut at Storrs acted as co-chair to Foss and helped in organizing the event.

Live demonstrations were ongoing by the software developers themselves, and hundreds of conference attendees viewed the packages, asked questions of the developers, and even "test drove" the fifteen packages on display during the three day event. The software,

designed for either IBM-compatible or Macintosh personal computers, included teaching aids for thermodynamics, kinetics, biochemical engineering, unit operations, process design, and process control.

Other software on display included numerical computation and network management packages which could be used throughout the chemical engineering curriculum. Software from the NSF Computer Modules Project was also presented. One committed developer, Professor Robert Squires of Purdue University, even brought his own Sun workstation so he could demonstrate his Simulation of Industrial Processes.

The computers were located in a specially designated area inside the registration area (Pasadena Room), where a schedule of demonstrations was posted. At any one time, several demonstrations were ongoing simultaneously throughout both the morning and afternoon sessions.

Given the success of the event, Groups 4 and 10 (Education and Computing and Systems Technology, respectively) have agreed to again co-sponsor a live demonstrations session at the 1992 AIChE Annual Meeting to be held in Miami this coming November.

Any academic interested in demonstrating either IBM PC or Macintosh compatible software they have developed specifically for educational purposes should send an extended abstract to both Douglas Cooper, Chemical Engineering Department, University of Connecticut, Storrs, CT 06269-3139, phone (203) 486-4092, and David Greenberg, Chemical Engineering Department, University of Cincinnati, Cincinnati, OH 45221-0171, phone (513) 556-2741. Please be certain to include hardware requirements for demonstrating the package.

Cray Research Joins the Engineering Design Research Center of Carnegie-Mellon University

Cray Research, Inc., the worldwide leader in providing high-performance computing solutions, has joined the Engineering Design Center (EDRC) of Carnegie Mellon University as an industrial affiliate. The EDRC is a multi-disciplinary National Science Foundation (NSF) engineering research center that develops and integrates computer-based methodologies to support more rapid, efficient, and cost-effective design in U.S. industry.

The EDRC spans all engineering disciplines, as well as architecture and computer science. The center operates on the premise that design practice can be dramatically improved at an early stage by applying formal methodology to enable designers to:

- Anticipate life-cycle concerns (e.g., manufacturing, testing, reliability)
- Convey thought processes that motivate design decisions
- Generate and select design alternatives automatically
- Develop design systems that are easy to learn and use

With its vision of improved design practice through advances in design science and computation tools, the EDRC's Industrial Affiliation Program has attracted substantial collaboration. Cray Research joins the EDRC industrial membership of 39 companies from the aerospace, computer, chemical, petroleum, automotive, medical equipment, construction, and materials industries.

"Collaborative projects with industry and academia are rapidly becoming the norm in our industry as a way of increasing the transfer of technologies," said John A. Rollwagen,

Chairman and CEO of Cray Research. "Our involvement with the EDRC not only provides the participating researchers with the resources to readily step into the world of high-performance computing, but also enables Cray Research to contribute to the advancement of engineering design. This partnership between industry and academia is a true win-win opportunity."

The EDRC research program is organized around three laboratories: design for manufacturing, synthesis, and design systems. The Design for Manufacturing Laboratory includes faculty from electrical, computer, and mechanical engineering disciplines, as well as architecture. Participants develop methodologies that enable designers to anticipate the downstream consequences of decisions they make while formulating a design.

The Synthesis Laboratory combines expertise from chemical, civil, and mechanical engineering, industrial administration, computer science, and architecture. Research teams develop and integrate qualitative and quantitative methods for design optimization in the areas of layout design, separation system synthesis, preliminary design of engineering systems, automated learning, and combinatorial optimization.

In the Design Systems Laboratory, architecture, chemical, civil, and electrical engineering combine to create generic design tools and domain-independent systems to support the large-scale integration of dissimilar design tools. A major goal of this laboratory is to create schemes for integrating designers, CAD tools, and modeling facilities in flexible organizations that support concurrent design.

Cray Research's current involvement is in the Synthesis Lab and Design Systems Lab. Future involvement is expected to extend to design for

manufacturing as well. Cray Research's membership with the EDRC is one of many formal and informal affiliations with universities and supercomputer centers throughout the U.S. Cray Research, Inc. designs, manufactures, markets, and supports large-scale, high-performance computer systems for scientific and engineering applications.

Chevron Affiliates with Pittsburgh Supercomputing Center

The Chevron Oil Field Research Company, a subsidiary of Chevron Corporation, has become a corporate affiliate of the Pittsburgh Supercomputing Center. The agreement enables Chevron researchers to complement their in-house supercomputing with access to the Center's facilities for high-performance scientific computing. Chevron will also have access to the Center's resources for training and consulting in the use of supercomputing technology.

Chevron scientists will use Pittsburgh's Connection Machine CM-2, one of a new generation of supercomputers that implements a design principle known as massive parallelism, to run computer simulations of underground oil and gas reservoirs. With the computing capability of the CM-2, Chevron scientists believe it will be possible to increase the size of their reservoir models by 10 times or more. This will permit the models to include more realistic geological information and thus to more accurately predict a reservoir's response to recovery schemes.

"Optimizing the recovery of known oil and gas resources," said Earnest

Chung, who leads Chevron's simulation research group, "is becoming more important as it has become harder and harder to find significant amounts of new oil in the United States." Increasing recovery from known oil fields in the United States by only one percent, for example, will yield more oil than the largest domestic oil discovery during the last decade, Prudhoe Bay in Alaska.

"We provide Chevron with a powerful, versatile set of computers that augment their in-house capability to design cost-effective recovery methods for oil," said Beverly Clayton, executive director of the Pittsburgh Supercomputing Center. "This is consistent with our mission, as charged by the National Science Foundation, to help American business use high-performance computing to enhance our competitive standing in the global marketplace."

In becoming a Corporate affiliate of the Pittsburgh Supercomputing Center, Chevron is joining other major American corporations, including ALCOA, USX, Pfizer Inc., DuPont, and Westinghouse, that rely on the resources of the Center as part of their Corporate research efforts.

The Pittsburgh Supercomputing Center, a joint project of Carnegie Mellon University and the University of Pittsburgh together with Westinghouse Electric Corporation, was established in 1986 by a grant from the National Science Foundation with support from the Commonwealth of Pennsylvania. Its purpose is to develop and make available state-of-the-art high-performance computing for scientific researchers nationwide.

Numerical Methods for Problems with Moving Fronts

by
Bruce A. Finlayson



An *essential* guide to methods
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Electronic Communications

ChE Electronic Newsletter

by *Martyn S. Ray*

More than 20 issues of the ChE Electronic Newsletter have already been published. Once again, CAST Communications brings this timely, convenient method of access to academic chemical engineering faculty to your attention. There is an approximate 3-month lag between the deadline for CAST newsletter material and the receipt of the newsletter by Division members. You can reduce this time lag to approximately one month by sending brief—maximum 12-15 lines if possible—announcements to Dr. Martyn Ray in Australia. As an example of the contents of the newsletter, items published in a recent issue include the following:

Volume 1, Issue Number 20, 1 December 1991

- Item 1. Symposium on Gas Separation by PSA
- Item 2. AIChE Separations Division (Newly Formed)
- Item 3. Call for papers: Product Recovery & Purification
- Item 4. Call for papers: Membranes for Bioseparation
- Item 5. Call for papers: Separating Contaminants from Groundwater
- Item 6. Low Cost Dissolved Oxygen Probes

The details of the electronic newsletter are as follows.

Editor: Dr Martyn S Ray, Senior Lecturer in Chemical Engineering,

Curtin University of Technology,
Perth, Western Australia. Phone: 09-351-7581; Fax: 09-351-2681
E-mail (Internet):
trayms@cc.curtin.edu.au,
ray_ms@cc.curtin.edu.au,
chemeng@cc.curtin.edu.au

1. Welcome. This is the 'n'th transmission of the ChE Electronic Newsletter (renamed from Chemical Engineering Digest, the 1st edition) via my E-mail chemical engineering mailing list. Please ignore the list of names that appear at the start of the message. I am working on removing these.
2. Please publicize the newsletter to colleagues (and students) who may be interested in joining the list.
3. Send BRIEF items—maximum 12-15 line—to the editor (trayms) for inclusion in the next issue. These can be requests for information or data, information on meetings and seminars, details of a new book to be published, discussion of a journal article, details of vacant faculty positions, sabbatical leave, etc.
4. We now have a chemical engineering news group (sci.engr.chem) on the net for general communications. This digest is for more important and specific items and goes direct to a targeted audience. Also at Curtin items are deleted from news groups after 7 days, the newsletter stays in your mailbox until read. Items may be included both in this newsletter and sci.engr.chem.
5. I have tried to reduce the line length as some sites were having problems.
6. ChE Electronic Newsletter back-issues available from ftp archive. To access the archive, ftp to cc.curtin.edu.au and login with a username of 'anonymous' and a

password of your name. If you look in the directory 'chemeng' (by typing `cd chemeng`) you will find an archive of back issues. Use the 'ls' and 'get' commands to list the files and retrieve them to your computer. Use 'quit' to finish.

Meetings, Conferences, Congresses, Short Courses, and Workshops

To submit a paper for consideration at any event listed below, please contact the corresponding session chairman or vice chairman directly. For further information or details about each of the four CAST Division programming areas, contact the appropriate Area Chairman as noted in the masthead. For general information concerning CAST Division sessions and scheduling, or to correct errors in this listing, please contact Jeffrey J. Sirola (CAST Division Programming Chairman), Eastman Chemical Company, P.O. Box 1972, Kingsport, TN 37662-5150, 615-229-3069, 615-229-4558 (Fax), sirola@kodak.com (E-mail).

New Orleans AIChE Meeting

March 29–April 2, 1992

The CAST Division is sponsoring the following sessions at the New Orleans National meeting:

Area 10a: Systems and Process Design

Session 57 (Monday AM). Process Modeling and Simulation I

Session 58 (Monday PM). Process Modeling and Simulation II

Session 59 (Tuesday AM). Integration of Process Design, Optimization, and Control

Session 60 (Tuesday PM). Training Simulators

Joint Area 10a and Area 10c Session:

Session 61 (Wednesday AM). Optimization of Batch Unit Operations

Area 10b: Systems and Process Control

Session 64 (Monday PM). Industrial Applications of Process Control

Session 67 (Wednesday PM). Plant Wide Control

Area 10c: Computers in Operations and Information Processing

Session 62 (Wednesday PM). Hazard and Operability Analysis

Session 63 (Monday AM). New Environments for Engineering Computations

Session 65 (Tuesday AM). Software Engineering Tools and Techniques I

Session 66 (Tuesday PM). Software Engineering Tools and Techniques II

IFAC Symposium on On-Line Fault Detection and Supervision in the Chemical Process Industries

Newark, Delaware
April 22–24, 1992

The program includes over 70 papers contributed by authors from industry and academia in more than 20 countries. Most of the technical sessions are followed by a discussion period. Poster sessions will complement oral presentations and will provide an opportunity for one-on-one discussions with authors. A wide range of industrial applications in process fault diagnosis, monitoring, supervision and control are included in both the poster sessions and the oral presentations. An exhibition of software and hardware vendors is planned in parallel with the meeting; it should provide attendees with the opportunity to become familiar with

state-of-the-art equipment and software. The Symposium is organized to provide excellent opportunities to exchange ideas and become acquainted with many of the active researchers and leaders in the field. The registration fee is \$350 before and \$400 after March 22, 1992.

For further information, please contact Professor Prasad Dhurjati, Dept of Chemical Engineering, University of Delaware, Newark, DE 19716.
Phone: 302-831-2979
Fax: 302-831-1048
E-mail: dhurjati@donald.che.udel.edu

3rd IFAC Symposium on Dynamics and Control of Chemical Reactors, Distillation Columns, and Batch Processes (DYCORD + '92)

College Park, Maryland
April 26–29, 1992

The Symposium will focus on three important areas of process dynamics and control: chemical reactors; distillation processes; and batch processes. Chemical reactors usually function at the heart of processing plants. They pose specific problems in start-up, run-away, stabilization, and hot-spot avoidance. Moreover, modeling is often difficult because of complicated and reaction kinetics and uncertain catalyst activity. Although well known, distillation processes are still difficult to control, particularly in view of today's stricter product purity requirements. The trend towards knowledge-intensive products has resulted in a re-examination of batch processes. Fortunately, modern distributed control systems offer an infrastructure for advanced automation and flexible operation. Specific topics are: flexibility, scheduling interlocking, and recipe handling. Apart from batch reactors and distillation processes, other batch

operations also fall within the scope of the Symposium.

The carefully selected program includes over 70 contributed papers covering all aspects of distillation, reactor, and batch control systems, from theoretical developments to practical applications. Five plenary and two tutorial speakers with international reputations have been invited to present keynote addresses on the state-of-the-art and future developments in the subject areas. The working language of the program is English. The registration fee is \$325 before and \$375 after March 1, 1992.

For further information, please contact the Registration Supervisor, DYCORD+'92, Center for Professional Development, Room 2101, University of Maryland, University College, University Blvd at Adelphi Road, College Park, MD 20742-1668. Phone: 301-985-7230. Fax: 301-985-7100.

8th Process Control Users Forum, Real Experiences in the Utilization of Technology

**San Antonio, Texas
April 27-29, 1992**

The Eighth Process Control Users Forum will give chemical industry process control engineers, systems engineers, process engineers, and process automation managers an opportunity to exchange non-proprietary information on trends, practices, and innovations in process automation. The theme of this forum is "Real Experiences in the Utilization of Technology" related to process control. Speakers and panelists will provide a chemical manufacturer's perspective on issues related to application of technology toward measurement, control, and process improvement. The Chemical Manufacturers Association's (CMA) Process Safety Code of Management

Practices will also be addressed by speakers who will discuss the use of safety technology to evaluate the performance of process control systems. Registration for the Eighth Process Control Forum is \$395 per person. To register, please notify CMA by the close of business, April 13, 1992. If you have registered and are unable to attend, please call 202-887-1283 by April 10, 1992. For further information, please contact Katie Quillen, Chemical Manufacturers Association, 2501 M Street, N.W., Washington, D.C. 20037. Phone: 202-887-1283. Fax: 202-887-1237.

European Symposium on Computer Aided Process Engineering (ESCAPE-1)

**Elsinore, Denmark
May 24-28, 1992**

ESCAPE-1 is a continuation of the series of events initiated by the EFChE (European Federation of Chemical Engineers) working party on Computer Aided Process Engineering (previously known as Use of Computers in Chemical Engineering). The most recent events in this series are CHEMDATA '88 at Gothenburg, CACHI '89 at Erlangen, COMCHEM '90 at the Hague and COPE '91 at Barcelona.

The subjects covered at this symposium will focus on the latest developments in computer applications relevant to chemical process engineering (including biochemical process engineering) in general and the following themes in particular:

- Process dynamics and process control
- Computer integrated process engineering
- New developments in the use of computers in chemical engineering
- Study of complex chemical processes

In addition, a workshop will be arranged immediately following the symposium on Process Simulation for Design and Operation of Chemical Processes.

For further information please contact:

ESCAPE-1
Engineering Research Centre IVC-SEP
Institut for Kemiteknik, Bygn. 229
The Technical University of Denmark
DK-2800 Lyngby, Denmark.
Tel: (45) 42883288 ext. 2830
Telefax: (45) 42882258
Telex: 37529 DTHDIA DK
BITNET: KETRG211@vm.uni-c.dk

NATO Advanced Study Institute, Batch Processing Systems Engineering

**Turkey
May 29-June 7, 1992**

This NATO Advanced Study Institute is to disseminate the proven scientific approaches to batch processing systems engineering and to further the systematic approach through advances such as mathematical programming, artificial intelligence, and computer science. Themes include: Design of multi-product, multi-purpose batch plants; Planning and scheduling of batch processes; Design and operating policies for complex batch units such as reactors and separators; Product design; Applications of batch processing in various chemical processing industries; Batch processing systems engineering under risk and uncertainty; Control and identification for batch processing; Mathematical programming techniques for batch processing, nonlinear optimization, and mixed-integer nonlinear programming; Artificial intelligence for batch processing, knowledge representation, machine learning through connectionist and symbolic

approaches; Discrete event simulation; and Batch process simulation software.

For further information, please contact: Aydin K. Sunol, ASI Director, Chemical Engineering Department, University of South Florida, 4202 E. Fowler Ave, Tampa, Florida 33620. Phone: 813-974-3566. Fax: 813-974-3561. E-mail: sunol@sunburn.ec.usf.edu

1992 American Control Conference

**Chicago, Illinois
June 24-26, 1992**

The following sessions have been developed by the CAST Division for the 1992 American Control Conference (ACC):

1. Modeling and Identification of Chemical Processes
2. Robust Process Control
3. Nonlinear Process Control
4. Model Predictive Control (Including Multi-Rate Control)
5. Batch Processes and Discrete Events
6. Pattern Recognition and Controller Performance Assessment
7. Intelligent Process Control

For further information, please contact:

Ali Cinar, Society Review Chair
Department of Chemical Engineering
Illinois Institute of Technology
Chicago, IL 60616
Phone: (312) 567-3042
Fax: (312) 567-8874
E-mail: checinar@iitvax

Martin Corless, Vice Chair for Contributed Sessions
School of Aeronautics & Astronautics
Purdue University
West Lafayette, IN 47907
Phone: (317) 494-7411
Fax: (317) 494-0307
E-mail: corless@gus11.ecn.purdue.edu

Advanced Process Systems Engineering: Concepts and Practice

**Engineering Design Research Center
Carnegie Mellon University
June 29-July 3, 1992**

This five-day course stresses the application of recently developed design concepts and optimization-based strategies to practical process problems. Geared to technical managers, industrial researchers and tool developers this course provides practical information and exposure to powerful modeling tools for process synthesis, analysis, optimization and planning.

Topics of this course include concepts for process synthesis (heat integration, separation systems, reactor networks), expert systems, modeling environments, flowsheet optimization, mixed-integer optimization models for process synthesis, strategies for retrofit design, differential algebraic systems, and planning and scheduling of batch processes. Course participants will learn about these topics through lectures and hand-on workshops making extensive use of powerful computer software (e.g. ASCEND, GAMS, SQP, DICOPT+). Also, a comprehensive set of lecture notes and handouts will be provided.

The instructors of the course are Professors Larry Biegler, Ignacio Grossmann, and Arthur Westerberg. The course will take place Monday through Friday, 8:30-5:00 and Friday

8:30-3:00. For information, please contact Ms. Tracy Farbacher, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213; Tel: (412) 268-6344 or Fax: (412) 268-7139.

Minneapolis AIChE Meeting

August 9-12, 1992

Although the CAST Division normally does not program at the Summer National Meetings, the Division is cosponsoring the following session with the Fuels and Petrochemicals Division.

Joint Area 10c and Area 16e Session:

1. High-Performance Computing in Chemical Science and Engineering. Stephen E. Zitney, Cray Research (Chairman) and Sangtae Kim, University of Wisconsin, (Vice Chairman).

CONTROL SYSTEMS '92 Dream vs Reality: Modern Process Control in the Pulp and Paper Industry

**Whistler, BC, Canada
September 28-October 1, 1992**

This Conference is part of a biennial series of control conferences held on even years alternately in Scandinavia and Canada. Control Systems '92, being held in Canada, is sponsored by the Technical Section, Canadian Pulp and Paper Association; and is co-sponsored by the Swedish association, Svenska Pappers-och Cellulosaingenieursforeningen, and the Finnish association, Suomen Paperi Insinööri Yhdistys Ry.

The Conference Chairman is Ron Crotagino and the Program Chairman is Alain Roche, both of Paprican,

Pointe Claire, Quebec. Our objective for this conference is to bring together control theorists, industry researchers and practitioners, and suppliers of control equipment to exchange ideas on what is needed to achieve "good" process control. The motivation for such a theme is that there is a growing mistrust of industrial users of control technology (at least in our industry) towards the theory developed in universities because this theoretical work is often perceived as being out of touch with the industrial reality. On the other hand, university researchers receive very little feedback from the industry. Consequently, only a very small fraction of the academic work finds its way into industrial application. We felt the time had come to organize a forum where people with very different perspectives could be given a chance to let other people know of their experience, realizations, and expectations.

A one-day workshop on modern modelling and control design techniques will be presented the day before the Conference by established experts in the field.

Additional information on the Conference can be obtained from:

David Paterson
Technical Section, CPPA
Sun Life Building, 19th Floor
1155 Metcalfe Street
Montreal, Quebec, Canada
H3B 4T6

Reply Form

Please return this form to:

Alain A. Roche, Program Chairman,
CONTROL SYSTEMS '92, The Pulp and
Paper Research Institute of Canada,
570 St John Boulevard,
Pointe Claire, PQ, H9R 3J9, CANADA

Please send me more information
about CONTROL SYSTEMS '92: _____

I am interested in attending CONTROL
SYSTEMS '92: _____

I am interested in attending the
workshop: _____

Name: _____

Address: _____

Tel. No.: _____

Fax No.: _____

Please also enclose the names and
addresses of any colleagues you think
might wish to be informed about this
conference.

Miami Beach AIChE Meeting

November 1-6, 1992

Meeting Program Chairman: James C.
Hill, Chemical Engineering
Department, Iowa State University,
Ames, IA 50011-2230. Phone: 515-294-
4959. Fax: 515-294-2689.

The CAST Division is planning the
following sessions at the Miami Beach
Annual Meeting. Deadlines and final
call for papers for this meeting appear
later in this issue.

Area 10a: Systems and Process Design

1. Process Systems Integration.
Babu Joseph, Washington University
(Chairman) and Michael L.
Mavrovouniotis, University of
Maryland (Vice Chairman).

2. Design and Analysis. Joseph F.
Pekny, Purdue University (Chairman)
and Amy R. Ciric, University of
Cincinnati (Vice Chairman).

3. Batch Process Engineering.
Heinz A. Preisig, University of New
South Wales (Chairman) and Michael

F. Malone, University of
Massachusetts (Vice Chairman).

4. Process Synthesis. Rakesh
Govind, University of Cincinnati
(Chairman) and D. Lionel O'Young,
Linnhoff March Inc. (Vice Chairman).

Joint Area 10a and Area 10b Session:

1. Design and Control.
Christodoulos A. Floudas, Princeton
University (Chairman) and William L.
Luyben, Lehigh University (Vice
Chairman).

Joint Area 10a and Area 10c Session:

1. Knowledge Based Systems.
Lyle H. Ungar, University of
Pennsylvania (Chairman) and James
F. Davis, Ohio State University (Vice
Chairman).

Area 10b: Systems and Process Control

1. Nonlinear Control. Vasilios I.
Manousiouthakis, University of
California, Los Angeles (Chairman)
and B. Wayne Bequette, Rensselaer
Polytechnic Institute (Vice Chairman).

2. Model Predictive Control.
James B. Rawlings, University of
Texas (Chairman) and Michael
Nikolaou, Texas A&M University (Vice
Chairman)

3. Advances in Process Control.
Evangelos Zafiriou, University of
Maryland (Chairman), Richard W.
Chylla, S. C. Johnson & Son, Inc. (Vice
Chairman), and Babatunde A.
Ogunnaike, E. I. du Pont de Nemours
& Co. (Vice Chairman).

**4. Modeling and Identification
Issues in Process Control.** Daniel E.
Rivera, Arizona State University
(Chairman) and Dominique Bonvin,
Institute d'Automatique, EPFL (Vice
Chairman).

**5. Process Monitoring and
Control.** Ali Cinar, Illinois Institute
of Technology (Chairman) and Venkat

Venkatasubramanian, Purdue University (Vice Chairman). **Joint Area 10b and Area 15c Session:**

1. Bioprocess Modeling, Monitoring, Optimization, and Control. Janice A. Phillips, Lehigh University (Chairman) and Tse-Wei Wang, University of Tennessee (Vice Chairman).

Area 10c: Computers in Operations and Information Processing

1. Advances in Optimization. Ignacio E. Grossmann, Carnegie Mellon University (Chairman) and Angelo Lucia, Clarkson University (Vice Chairman).

2. Parallel Computing. Stephen E. Zitney, Cray Research Inc. (Chairman) and Anthony Skjellum, Lawrence Livermore National Laboratory (Vice Chairman).

3. Progress in Computer Integrated Manufacturing in the Chemical Process Industries. (Cosponsored by the International Cooperation Committee of the Society of Chemical Engineers, Japan) Iori Hashimoto, Kyoto University (Cochairman) and G. V. Reklaitis, Purdue University (Cochairman).

Area 10d: Applied Mathematics and Numerical Analysis

1. Characterization, Modeling, and Analysis of Process Systems with Complex Dynamics. B. Erik Ydstie, University of Massachusetts (Chairman) and Julio M. Ottino, Northwestern University (Vice Chairman).

2. Analysis of Complex Systems. Ioannis G. Kevrekidis, Princeton University (Chairman) and Hseuh-Chia Chang, University of Notre Dame (Vice Chairman).

3. Optimization: Theory and Algorithms. Joseph F. Pekny, Purdue University (Chairman) and Ross E. Swaney, University of Wisconsin (Vice Chairman).

4. Geometric and Similarity Methods for Nonlinear Analysis in Engineering. Jeffrey C. Kantor, University of Notre Dame (Chairman) and Michael F. Doherty, University of Massachusetts (Vice Chairman).

5. Applied Mathematics and Computer Methods. George D. Byrne, Exxon Research and Engineering Company (Chairman) and Bruce Finlayson, University of Washington (Vice Chairman).

In addition to technical sessions, CAST will also cosponsor with Area 1 and Area 4 the second annual Educational Software Demonstrations. These will be organized by Douglas J. Cooper, University of Connecticut (Chairman) and David Greenberg, University of Cincinnati (Vice Chairman).

Houston AIChE Meeting

March 28–April 1, 1993

Meeting Program Chairman: Robert F. Dye, Dye Engineering and Technology Co., 3011 Fairway Dr., Sugar Land, TX 77478. Phone: 713-494-5617. Fax: 713-494-0210.

The CAST Division is planning the following tentative program at the Houston National Meeting. AIChE and the Meeting Program Chairman will finalize the sessions at the 1992 Programming Retreat in February, and any corrections will appear in the next issue of CAST Communications. Tentative deadlines and first call for papers for this meeting appear later in this issue.

Area 10a: Systems and Process Design

1. Retrofit Design Techniques and Applications. Vivek Julka, Union Carbide Corporation (Chairman) and Jeffrey P. Knapp, E. I. du Pont de Nemours & Company (Vice Chairman).

2. New Advances in Process Synthesis and Analysis. Amy R. Ciric, University of Cincinnati (Chairman) and Mahmoud El-Halwagi, Auburn University (Vice Chairman).

3. Industrial Applications of CAD. R. L. Motard, Washington University (Chairman) and Herbert I. Britt, Aspen Technology Inc. (Vice Chairman).

Joint Area 10a and Area 10c Session:

1. Design for Operability. John T. Baldwin, M. W. Kellogg Company (Chairman) and Mark Fligner, Mobil R&D Corporation (Vice Chairman).

Joint Area 10a and Area 11 Session:

1. Design for Safety and Environmental Impact. Amy R. Ciric, University of Cincinnati (Chairman) and Brian J. Tarantino, Merck & Company, Inc. (Vice Chairman).

Joint Area 10a and Area 15 Session:

1. Bioprocess Design and Simulation. Paul C. Chan, Aspen Technology (Chairman) and James G. Stramando, Biotechnology Consultant (Vice Chairman).

Area 10b: Systems and Process Control

1. Industrial Applications in Process Control. Gerardo Mijares, M. W. Kellogg (Chairman) and J. Kirk Bailey, Sunoco (Vice Chairman).

2. Nonlinear and/or Predictive Control in Practice. Robert B. Hawkins, Dynamic Matrix Control (Chairman).

Area 10c: Computers in Operations and Information Processing

1. Promise of Integration. Jerry L. Robertson, Exxon Research and Engineering (Chairman) and Stephen

J. Zilora, Creative Software Solutions (Vice Chairman).

2. Integration of Planning and Scheduling. C. E. Bodington, Chesapeake Decision Sciences (Chairman) and J. Kirk Bailey, Sunoco (Vice Chairman).

3. Process Modeling and Optimization. Michael C. Wellons, Mobil R&D Corporation (Chairman) Iauw-bhieng Tjoa, Dynamic Matrix Control (Vice Chairman).

4. Experiences with Real-time Packages. F. Eric Finch, Gensym Corporation (Chairman) and Subodh Ganguly, Mobil R&D Corporation (Vice Chairman).

5. Integration of Simulation and Operations. Richard D. LaRoche, Cray Research Inc. (Chairman) and Alan B. Coon, Union Carbide Corporation (Vice Chairman).

Area 10d: Applied Mathematics and Numerical Analysis

No Sessions are planned.

Foundations of Computer-Aided Process Operations (FOCAPO '93)

**Mount Crested Butte, Colorado
July 18-23, 1993**

Cosponsored by CAST Division and CACHE Corporation.

The second Foundations of Computer-Aided Process Operations conference is scheduled for summer 1993. The technical program is expected to include sessions on Optimal Scheduling and Planning, Computer Integrated Manufacturing, Interface with Process Design and Control, Data Management, Knowledge Representation, Impact of High Performance Computing, Human Factors in Process Operations, and other topics.

For more information, contact David W. T. Rippin (Conference Chairman), Chemical Engineering Department, Swiss Federal Institute of Technology, ETH Zentrum, CH-8092 Zürich, Switzerland, 01-256-3112 or John C. Hale (Conference Vice Chairman), E. I. du Pont de Nemours & Company, P.O. Box 6090, Newark, DE 19714-6090, 302-366-3041, 302-366-4889 (Fax).

St. Louis AIChE Meeting

November 7-12, 1993

Meeting Program Chairman: James R. Deam, Monsanto Company - F2WG, 800 North Lindbergh Blvd., St. Louis, MO 63167. Phone: 314-694-6061. Fax: 314-694-6138.

The CAST Division is considering the following programming topics for the St. Louis Annual Meeting. AIChE and the Meeting Program Chairman will finalize the sessions at the 1992 Programming Retreat in February, and the approved program will appear in the next issue of CAST Communications.

Process Synthesis

Synthesis of Complex Separation Systems

Design and Analysis

Design Under Uncertainty

Advances in Process Control

Identification and Adaptive Control

Nonlinear Control

Model Predictive Control

Robust Control

Enhancement of Process Safety and Environmental Protection through Process Control

Solutions to the Industrial Challenges in Process Control

Modeling and Control of Polymerization Processes

Real-Time Optimization and Plant-Wide Control

Information Systems in Design

Computational Approaches in Complex Engineering Systems

Statistical Tools in Process Operation

Plant Wide Dynamic Simulation

Data Interpretation

Artificial Intelligence in Process Engineering Visualization

Computer Integrated Manufacturing

Parallel Numerical Methods and Applications

Foundations of Computer-Aided Process Design (FOCAPD '94)

Summer 1994

The fourth International Conference on Foundations of Computer-Aided Process Design is tentatively scheduled for Summer 1994. The conference organizers and a preliminary outline of the technical program will be announced in the next newsletter.

Call For Papers

Special Announcement for Cosponsored Session Minneapolis AIChE Meeting August 9-12, 1992

Joint Area 10c and Area 16e Session

1. High Performance Computing in Chemical Science and Engineering

Recent and projected advances in high-performance computing technology pose grand challenges as well as offer great rewards to the chemical engineering "computational" community. This session will bring together researchers from diverse branches of chemical engineering who share a common vision that high-performance computing is a powerful research tool for generating new insights and breakthroughs in their disciplines. Papers are solicited in computational chemistry, computational fluid dynamics, chemical process engineering, and other application areas for high-performance computing in chemical science and engineering.

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Final Call for CAST Sessions Miami Beach AIChE Meeting November 1-6, 1992

The names, addresses, and telephone numbers of the session chairmen are given on the next several pages, as are brief statements of the topics to receive special emphasis in selecting manuscripts for these sessions. Prospective session participants are encouraged to observe the following deadlines, which however, may be changed at any time by the Meeting Program Chairman:

April 1, 1992: Submit an abstract (typically 300-500 words) and Proposal-to-Present Form to the session chairman and preferably a copy also to vice chairman.

May 1, 1992: Authors informed of selection and session content finalized.

August 1, 1992: Submit an extended abstract (camera-ready on a form to be provided for publication and distribution at the meeting) to the session chairman.

October 1, 1992: Submit final manuscript to AIChE.

Area 10a: Systems and Process Design

1. Process Systems Integration

Papers are sought in the area of process systems integration. Specific topics of interest include design and control of integrated process units, integrated approaches to waste treatment and environmental issues, software for facilitating process systems integration, and theoretical issues in the design and operation of large integrated process systems.

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2. Design and Analysis

This session will address recent developments in process design and analysis. Session topics include, but are not limited to, systematic approaches and shortcut heuristics for process synthesis, new models of specific unit operations and processes, innovations in analysis techniques, advances in design education and design philosophy, and developments

in supporting numerical methods. An emphasis will be placed upon presentations of interest to a broad audience.

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3. Batch Process Engineering

Papers are solicited reporting on progress in the design and operation of batch processes. The session is not limited to the discussion of a particular aspect, but preference will be given to papers that contribute to the integration of design and operation. Studies of robust design, which accounts for uncertainties in various parts of the overall model such as equipment, planning schedule, utilities, and product market are also of interest.

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4. Process Synthesis

Papers dealing with fundamental research and/or successful applications in the field of process synthesis are welcome. This includes synthesis of systems such as reactors, separators, heat and power recovery, or other unit operations. The theory or application of the techniques could be for grassroot designs or retrofit problems. Topics of interest include, but are not limited to, recent advances in the optimization of large-scale systems involving multiple types of unit operations or multiple objectives, application of advanced reasoning techniques for process synthesis applications, and application of process synthesis techniques to industrial problems.

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Joint Area 10a and Area 10b Session:

1. Design and Control

Papers are solicited describing novel methodologies, modeling issues, applications, and case studies for the integration of process design and control. Topics of interest include, but are not limited to process synthesis based approaches that introduce operability (e.g., controllability, flexibility, robustness, reliability) measures at early stages of design, theoretical and modeling frameworks that establish the tradeoff between design and control, and industrial applications demonstrating the impact of design and/or control modifications on integrated processes.

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Joint Area 10a and Area 10c Session:

1. Knowledge-Based Systems

Papers studying the use of knowledge-based expert systems and artificial intelligence in chemical engineering are solicited. Applications of AI to problems in process operations, including process fault detection, diagnosis, and control are sought, as are methodological contributions such as novel knowledge representation or reasoning techniques.

Chairman

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Area 10b: Systems and Process Control

1. Nonlinear Control

Papers are solicited in all areas of nonlinear process control. Topics of interest include differential geometric-based approaches, nonlinear optimal control, nonlinear robust control, reference systems synthesis, sliding mode control, and control of systems with saturation.

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2. Model Predictive Control

Papers which demonstrate advances in model predictive control theory or applications are invited. Topics of particular interest include input and output variable constraints, nonlinear model-based control, robustness with respect to structured and unstructured uncertainties, nonsquare systems, and multirate sampling.

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3. Advances in Process Control

Papers in all areas of process control are sought. Priority will be given to papers that emphasize recent developments, novel applications or the definition of new problem areas. Papers from industrial contributors are especially welcome.

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Vice Chairman

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4. Modeling and Identification Issues In Process Control

This session is focused on the problem of modeling and identification of dynamic models for process systems, with emphasis on issues that affect the subsequent task of control system design. Both theoretical and application papers are sought in the areas of selection of model structure, complexity and parsimony, model validation and uncertainty estimation, design of experiments for identification, identifiability and sensitivity of model prediction with respect to parameters, black-box, grey-box, and mechanistic modeling, modeling requirements for process control, and modeling of partially known systems. Papers focusing on techniques that make the task of modeling and identification more amenable to practicing engineers are especially welcome.

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5. Process Monitoring and Control

Abstracts are sought on papers that address the interface of process monitoring and control including techniques and tools for monitoring process performance or control system performance by utilizing system theoretic, artificial intelligence and/or statistical approaches, integrated techniques and tools that coordinate monitoring and control activities, and case studies.

Chairman

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Joint Area 10b and Area 15c Session:

1. Bioprocess Modeling, Monitoring, Optimization, and Control

Biotechnology has become increasingly important in the production of food, pharmaceuticals, and agricultural products. Yet, due to the biological nature involved in the processes and the lack of on-line sensors, the modeling, monitoring, optimization, and control of such processes still remain a formidable challenge. A better modelling of the processes, development of sterilizable on-line sensors for extracellular components, appropriate control algorithms for taking care of process characteristics such as nonlinearity and model uncertainties will all greatly improve the optimization of bioprocesses. This session will welcome reports of recent developments within these areas of interest.

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Area 10c: Computers in Operations and Information Processing

1. Advances in Optimization

The goal of this session is to present theoretical and computational developments in optimization algorithms,

applications, and computer software. Topics of interest include large-scale linear and nonlinear programming, integer and mixed-integer programming, differential-algebraic optimization, and global optimization. Applications of interest include steady-state and dynamic models for design, and planning and scheduling. Industrial applications and computational experience with new techniques for optimization are also welcome.

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2. Parallel Computing

With the development of faster computers and new architectures that enable parallel processing, computational chemical engineering is in the state of rapid development. This session will focus on new developments in the use of shared and distributed memory supercomputers, massively parallel systems, and distributed networks of machines to solve large-scale chemical engineering problems. Topics of particular interest include new applications of parallel computing, parallel numerical algorithms, software engineering issues, performance analysis, scientific visualization, and networks and communications.

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3. Progress in Computer Integrated Manufacturing in the Chemical Process Industries

Contributions are sought describing methodological developments, implementations, and experiences with all aspects of CIM in the process industries. Subjects of particular interest include: integration of application areas such as plant information systems, monitoring, diagnosis, control, scheduling/optimization, and planning as well as

developments within these application areas themselves. Presentations of industrial experiences with CIM technology and critical discussions of limitations/advantages of current developments are also welcomed.

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Joint Area 10c and Area 5d Session:

1. Managing Information in the 90s

This session, cosponsored by the Management Division, will address the emerging technologies of computer hardware and software as they change the nature of storage, retrieval, and the use of information from the point of view of the end user of the information. The paper should address the information architecture and solution applied to a specific business process, e.g., engineering, R&D, production management, etc. Presentations may include topics such as information services, repository and data management, end user tools, client/server HW/SW solutions, etc., but they are expected to focus primarily on the application of this technology to solving the business process through better information management, access and analysis. Both technical and user oriented papers will be accepted.

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Area 10d: Applied Mathematics and Numerical Analysis

1. Characterization, Modeling, and Analysis of Process Systems with Complex Dynamics

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2. Analysis of Complex Systems

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3. Optimization: Theory and Algorithms

This session addresses the use of optimization methods in engineering and new developments in optimization. Submissions are especially encouraged for applications in engineering analysis, theoretical advances, new algorithms, global methods, strategies to exploit problem-specific structure, and computational experience associated with any of these areas.

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4. Geometric and Similarity Methods for Nonlinear Analysis in Engineering

This session is to review the established role of geometric similarity methods in mechanics and engineering analysis, and to survey the emerging role of these techniques in nonlinear process control and analysis.

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5. Applied Mathematics and Computer Methods

This session focuses on mathematical methods used to solve engineering problems, especially those which use the computer. Papers should include information on the algorithm and its performance. The applications are to be from the field of chemical engineering.

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First Call for CAST Sessions Houston AIChE Meeting March 28-April 1, 1993

The names, addresses, and telephone numbers of the session chairmen are given on the next several pages, as are brief statements of the topics to receive special emphasis in selecting manuscripts for these sessions. Prospective session participants are encouraged to observe the following deadlines which have been established, but may be changed, by the Meeting Program Chairman:

September 15, 1992: Submit an abstract (typically 300-500 words) and Proposal-to-Present Form to the session chairman and preferably a copy also to the vice chairman.

October 1, 1992: Authors informed of selection and session content finalized.

January 15, 1993: Submit an extended abstract (camera-ready on a form to be provided for publication and distribution at the meeting) to the session chairman.

February 15, 1993: Submit final manuscript to AIChE.

Area 10a: Systems and Process Design

1. Retrofit Design Techniques and Applications

Papers submitted for this session should describe design techniques and methodology for retrofitting plants, and/or experiences in process retrofitting and how retrofit design techniques were used to identify process improvements. The process improvements achieved might be in areas such as improved raw material efficiency, waste minimization, reduced energy consumption, increased capacity, improved product quality, or improved process flexibility. Algorithms and procedures and their embodiment in computer software can be described provided that the focus is on the chemical engineering technology and not on the mathematical procedures or the features of the software.

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2. New Advances in Process Synthesis and Analysis

Papers are solicited that report upon recent progress in process synthesis and analysis. Session topics include, but are not limited to, new models of unit operations, short-cut design heuristics, systematic design methods, innovative analytical and numerical methods, unusual applications of existing design methods, and advances in design education and design philosophy.

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3. Industrial Applications of CAD

Topics of interest include novel applications of Computer-Aided Design software, support of operating environments, design of unconventional systems, use of very large scale simulators and models, use of simulators in data reconciliation, fine tuning of processes and retrofit studies using CAD, and CAD in distributed computing environments.

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Joint Area 10a and Area 10c Session:

1. Design for Operability

This session is intended to address the design issues for the successful operation of processing plants viewed from a computing and systems technology vantage point. Issues of this view include the flexibility, controllability, and information flow of the system. Another aspect of operability is the recognition that processing plants have a life cycle that includes conceptualization, design, construction, operations, upgrades and revamps, and decommissioning. It would be appropriate to include design considerations based on this observation in the discussions. The focus of the session will be on the computing methods and tools that are used during the design activity that will

provide insight into the operability of processing plants. It is desired to have input from academia, design functions, process control functions, and plant operations functions in order to cover the subject matter.

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Joint Area 10a and Area 11 Session

1. Design for Safety and Environmental Impact

Safety and environmental friendliness often go hand-in-hand. Industrial accidents may involve fires or unintentional releases that can seriously damage or pollute the natural environment, and fugitive emissions that endanger the environment may also be health or fire hazards. This session will explore the common features of safe chemical processes and environmentally friendly chemical processes. Topics for discussion include, but are not limited to, improved process reliability, environmental impact assessments of chemical process accidents, equipment and process design for reduced fugitive emissions, and applications of safety analysis measures to waste reduction. Papers discussing case studies, combined safety and waste-minimization studies, and new design and analysis methods are welcome.

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Joint Area 10a and Area 15 Session

1. Bioprocess Design and Simulation

Flowsheet simulation, an invaluable tool in the chemical process industry, is being increasingly used in the biomanufacturing area for process design, development, optimization, and economic feasibility analysis. We are soliciting papers that describe experiences in the application of simulation to biological processes, either as an off-line tool for process development or as an on-line aid in process

operation and control. Papers dealing with integrated batch, semibatch, semicontinuous, and cyclic bioprocesses in the areas of fermentation, cell culture, or downstream recovery are particularly welcome. Papers that describe novel experiences in industrial applications of bioprocess simulation tools are also solicited.

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Vice Chairman

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Area 10b: Systems and Process Control

1. Industrial Applications in Process Control

Papers are requested on topics relating to the industrial application of advanced process control methods. Desirable areas include predictive model-based control, nonlinear model-based control, constraint control, adaptive control, and robust control systems.

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2. Nonlinear and/or Predictive Control in Practice

Papers are solicited reporting on the application of nonlinear or model-based predictive control techniques to real problems. Priority will be given to papers that discuss the practical issues arising from the application of these kinds of controllers, or that describe actual control application design or commissioning experience. Other topics of interest include performance monitoring, tuning, and modelling issues unique to non-linear or predictive controllers.

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Area 10c: Computers in Operations and Information Processing

1. Promise of Integration

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2. Integration of Planning and Scheduling

Planning is the forecasting of process or plant operations over a discrete time horizon of weeks, months, or years. Scheduling forecasts operations, inventories, etc. over a very short time horizon of hours, days, and weeks. Papers are solicited on the integration of these two functions, either in practice, or as a result of research, so that the plan and schedule are near optimum relative to the long term plan of the enterprise.

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Vice Chairman

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3. Process Modeling and Optimization

Papers are sought in all areas of process modeling and optimization. Contributions that address applications to industrial processes for process monitoring, off-line planning, and on-line optimization are particularly welcome.

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4. Experiences with Real-time Packages

This session will focus on innovative real-time applications implemented using commercial or in-house software packages. Emphasis will be on industrial experience with on-line systems. Application areas include, but are not necessarily limited to, statistical process control, real-time scheduling and planning, process monitoring, neural networks, expert systems, and diagnosis.

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Vice Chairman

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5. Integration of Simulation and Operations

This session addresses issues arising from the integration of chemical process simulation and plant operations. These issues include, but are not limited to, the design, implementation, and modification of component software packages for use in such an integrated environment. Among the desired features of such software candidates are flexibility, computational efficiency, and ease of integration into existing distributed control or data acquisition systems, as well as various process engineering databases. These integrated environments may also involve the use of knowledge-based systems in either advisory or real-time model-based control. Descriptions of such software components, for example simulation, control, optimization, scheduling, etc., or their application are sought for this session, along with descriptions or case studies of their implementation and impact on plant operations.

Chairman

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