Computing and Systems Technology Division Communications

Volume 14, Number 2, Summer 1991

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About This Issue

by Peter R. Rony and Joseph D. Wright

As is becoming the tradition, the summer issue of CAST Communications features contributions from industry, in this case articles on "Chemical Process Synthesis, Design, and Operations Using Supercomputers," by Stephen E. Zitney and Richard D. LaRoche of Cray Research, and "Object Oriented Programming," by Ron Fosner of Lotus. Ron's contribution was a direct consequence of our solicitation for a contribution on object-oriented software. In a forthcoming issue, we shall publish a second article (by Dennis L. Brandl) on this subject, in the context of batch process control system design software.

Readers of this issue may observe a bit of streamlining in the publication of AIChE programming information, including both sessions and Calls for Papers. At the recommendation of Jeff Siirola, Programming Chairman, we have decided to minimize duplication and save page costs.

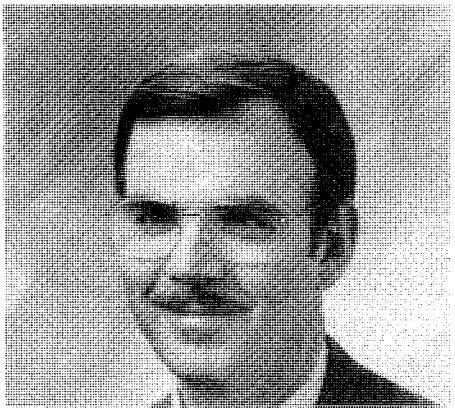
Though the Calls for the Automatic Controls Conference (ACC '92) are disseminated with a first deadline that barely precedes the publication date of this letter, we have decided to print the Calls so that Division members can develop insight into the sessions to be held next summer.

We congratulate our three 1991 CAST Division award winners, and extend an invitation to each of them to continue our publication tradition by contributing a feature article to the Winter 1992 issue of the newsletter.

We look forward to seeing many of you at the CAST Division Dinner on Tuesday, November 19, 1991. The CAST Executive Committee extends an invitation for all of you to attend.

CAST Division 1991 Chairman's Message

by G. V. Reklaitis



With this note, it is my pleasure to appraise the Division membership of some of the activities and plans of the Division since the 1990 annual meeting.

Of course, the most important Division function is programming at the regularly scheduled meetings of the Institute and at international meetings which the Division cosponsors. The Division organized 10.5 sessions at the Spring National Meeting, 5 sessions at the Summer National Meeting, and 26 at the Annual Meeting in Los Angeles to be held in November. The two specialist meetings of which the Division was cosponsor, the Chemical Process Control IV Conference held on South Padre Island in February and the Fourth International Symposium on Process Systems Engineering held at Montebello, Quebec in August were notable successes. The timing for the next Foundations of Computer Aided Plant Operations meeting has been deferred to the Summer of 1993. These events have been effectively planned under the leadership of the Programming Board, chaired by Jeff Siirola, and professionally executed as a result of the efforts of a host of session chairs, co-chairs, and authors. The Executive Committee commends these many individuals for their sterling volunteer efforts and would like to encourage all Division members to become involved in sustaining the Division's superlative reputation for programming excellence.

A complementary and equally important function of the Division is its newsletter, CAST Communications. Under the diligent efforts of Editor Peter Rony and co-Editor Joe Wright, a very fine issue was distributed to the membership last Spring and of course this the Fall issue again attains the high standards that these colleagues have established and sustained. The Executive Committee is very grateful of the leadership shown by Peter and Joe and appreciates the contributions of the authors who have provided manuscripts and newsworthy material. We would strongly encourage potential contributors to contact the Editors to discuss and submit interesting materials for possible publication.

Finally, this year the Executive Committee has launched a comprehensive long range planning activity which seeks to develop objectives for the growth and progress of the Division and to generate new ideas and initiatives through which to achieve these objectives. Beginning with a working meeting held at the Houston Meeting, the Executive Committee has been evolving a draft document which will be fully discussed at the Executive Committee meeting on Monday evening, November 18, at the Los Angeles Meeting. While it is premature to present the full details of this planning document at this time, I will summarize a few of the action items under consideration so as to obtain some feedback and stimulate further ideas from you.

As you know, the mission of the Division is to further the application of mathematical and computing principles in chemical engineering, particularly with respect to analysis, design, and control of process and management systems. There are seven

areas of activity of the Division which are being examined carefully to establish goals and devise initiatives which will allow these goals to be realized over the next five years. These are: programming and meetings, publications, membership, international and intersociety relations, finances, outreach within AIChE, and awards. Initiatives which are under discussion include:

- sponsorship of a specialty conference by the Applied Mathematics and Numerical Analysis programming area
- specific steps to improve the quality of CAST sessions and presentations
- efforts to simplify the processing of abstracts and session related forms
- elimination of the Speaker's Breakfast and its replacement with a more effective informational forum for first time speakers
- search for corporate sponsorship of advertisements and student special issues of the newsletter
- opening CAST Communications for subscription by non-AIChE members
- mechanisms to increase the number of BS level members
- an increase in the Division dues to levels more comparable to those of other active divisions
- efforts to help the national office in exploiting computer technologies to streamline meeting planning, communications, and arrangements
- fundraising to seek endowments for the Division awards and to raise the financial level of the awards

In regards to the third item, the Division First Vice-Chair, Ignacio Grossmann, discussed CAST Executive ideas for simplifying the proposal to present and abstract submission process at the Pittsburgh meeting of the Council of Division Officers. The ideas met with strong approval and a proposal is now being formulated by the Executive Committee for presentation to Council. The elimination of the Speaker's Breakfast also received positive reception and alternate, more cost-effective mechanisms are now under consideration. On the matter of the Division dues, at present 90% of the income from membership dues are expended on newsletter publishing costs (the editors and writers are all unpaid volunteers). With the present dues level of $7, the Division simply has no funds to undertake any other activities, even as simple as publication of a membership directory. An increase to say $10 would provide much needed flexibility for new initiatives.

On behalf of the Division Executive Committee, I would like to solicit the opinions and comments of the Division membership on these and any other issues that are appropriate for consideration as part of the Division's plans for the future. Please transmit your suggestions to me or any member of the Executive. We will be delighted to pursue them and, if timely and appropriate, to present them for consideration at our next meeting. This is an organization that exists and functions only as a result of the efforts of active and concerned volunteers. We have a lot to contribute to the profession and the industry. Join in!

Finally, I do hope to see you all at the Division awards banquet and annual meeting in Los Angeles on Tuesday evening, November 19. Come meet the award winners, the officers and fellow members and discover how wonderful rubber hotel banquet chicken can be.

An Invitation to Attend the CAST Division Awards Banquet

Members of the CAST Division, and their spouses and colleagues, are invited to attend the CAST Division Dinner in the Bonaventure Hotel, Santa Anita C room on Tuesday, November 19, 1991 at the Los Angeles National AIChE meeting. A cash bar starts at 7:00 p.m.; dinner commences at 8:00 p.m. The ticket price is $45.

The dinner is the one formal occasion during each year when CAST members gather socially and is always a very pleasant occasion. Rudolphe Motard, recipient of the 1991 Computing in Chemical Engineering Award, will deliver his award address. Jeffrey Siirola and Michael Mavrouniotis will receive the 1991 Computing Practice Award and the 1991 Ted Petersen Student Paper Award, respectively.

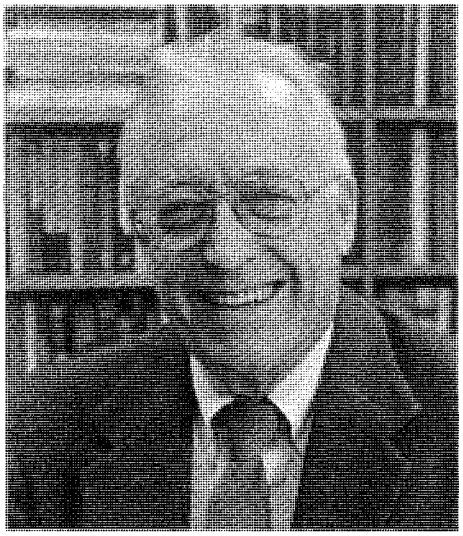
An Invitation to Attend the CAST Division Executive Committee Meeting

The CAST Executive Committee extends an invitation to members of the Division to attend the Fall Executive Committee meeting as well as the Area Programming meetings (consult the committee meeting listing at the registration desk for times and locations, since none will have been set by the publication date of this newsletter). All four areas will be planning their 1993 programming.

The CAST Executive Committee would like to encourage Division members to develop greater association with the Division, if not the Institute as a whole. We would that you feel that your needs are being served, and that your personal participation counts.

Awards

Rudolphe Motard is the Recipient of the 1991 CAST Division Computing in Chemical Engineering Award



For his pioneering research activities and for work that has significantly impacted industrial practice, Dr. Rudolphe Motard, Chairman of the Department of Chemical Engineering at Washington University and Director for the Center for Computer Aided Process Engineering, will receive the 1991 CAST Division Computing in Chemical Engineering Award at the CAST Division banquet on Tuesday evening, November 19, 1991, at the Los Angeles AIChE meeting.

The supporting statement for his award includes the following:

Professor Motard is one of our pioneers in computer-aided systems engineering in chemical engineering. If anything characterizes his contributions to this area, it is his ability to examine difficult systems problems and to discover remarkably simple ways to approach and solve them.

In the late 1960s, he and his students created the Chemical Engineering Simulation System (CHESS), a flowsheeting package that was distributed to over 100 academic institutions worldwide and which became the basis of two industrial flowsheeting systems. Creating this package inspired his research into convergence acceleration methods for flowsheeting systems, and to three significant contributions to algorithms to establish the sequence in which unit models are executed when they form a computational recycle. The first contribution—often referred to as the Barkley-Motard algorithm, reversed the role of links and nodes in the process graph and allowed for the discovery of a very effective set of graph reduction manipulations that greatly simplified the finding of desirable computational orderings [Barkley and Motard, 1972]; the second contribution used insights about the Upadhye and Grens ordering approach to produce an algorithm that is the basis of the current ordering algorithm in the ASPEN flowsheeting package [Westerberg and Motard, 1981]; and the third contribution is the use of these same insights to develop orderings that repeat units in order to improve convergence.

The work with Mahalec in the early 1970s on flowsheet synthesis provided what may still be the only approach of consequence for solving the seemingly innocuous general separation problem originally posed by Rudd, Siirola, and Powers in the late 1960s [Mahalec and Motard, 1977a and 1977b]. It was based on the resolution principle to synthesize total flowsheets (and within such a problem, to synthesize separation systems). His work with Agnihotri presented a method to enumerate all the chemical species that could form if certain types of species were mixed in a reactor [Agnihotri and Motard, 1980]. Testing was done on the basis of thermodynamics. This work was to aid in the design of catalysts to enhance the formation of desired products and inhibit undesired products.

Professor Motard's work with Nath was among the first, if not the first, to consider non-sharp separation problems [Nath and Motard, 1981]. This work provided the Material Allocation Diagram (MAD), a very useful representation for such a problem that has subsequently been used by others in their work.

With Su, Rudy provided one of the early effective algorithms for synthesizing heat exchanger networks [Su and Motard, 1984]. A significant idea in this work was a loop-tearing algorithm that allowed one to remove quickly extra heat exchangers from a network. This algorithm became the basis of a simulation algorithm within Simulation Science's HEXTRAN software system.

Of late, many researchers in process systems engineering are looking into concept representation as an important issue in the creation of CAD tools. Again displaying his pioneering spirit, Rudy was one of the first in the ChE research community to work on such problems by looking into the use of data bases to support modeling and simulation [Blaha et al, 1985 and Motard, 1986]. He became one of the first among us to converse expertly about inheritance and object-oriented modeling.

Supporting statements on behalf of his candidacy included:

"There is no question in my mind that Rudy has been one of the pioneers and leading figures in the area of process simulation, process synthesis, and computer-aided engineering. His work has greatly influenced other academic

researchers, and has had several industrial applications."

"Rudy is widely known for his work on the CHESS process simulator, one of the earlier packages in the area, which was disseminated to many academic institutions. This provided, for the first time, exposure of a process simulator to undergraduate students of chemical engineering. This work also promoted the study of tearing and convergence techniques for recycles. Here Rudy made outstanding contributions, as for instance the Barkley- Motard algorithm, which motivated many current implementations of tearing methods in commercial process simulators. Also, his review paper in AIChE J. in 1975, with Shacham and Rosen, has become one of the classic papers in the area. Subsequently in 1979, he was coauthor of the book, "Process Flowsheeting," which presented the most comprehensive and up-to-date treatment of the subject."

"His resume provides ample evidence of his numerous important contributions. In the following statements I would like to concentrate on a few which I hold in particular high esteem:

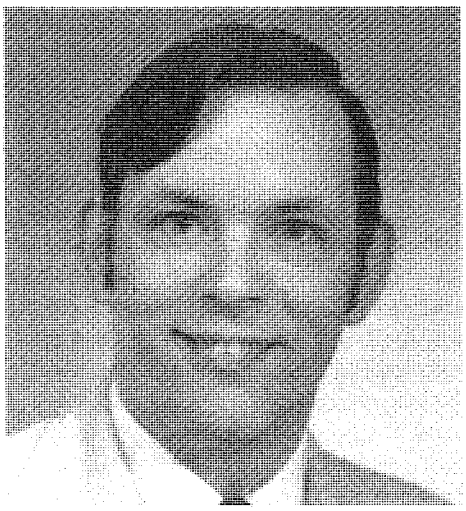
- In Rudy's pioneering work with Mahalec we see the first application of theorem-proving techniques from artificial intelligence to the problem of an initial design of a chemical processing system. I am ever anew excited by the clean problem formation presented in this work.

- In the paper with Agnihotri, new techniques for reaction path synthesis are proposed that profoundly influenced future work in this area.

- The 'loop-breaking' technique with Su was the basis of ideas on how to simplify computer-generated heat exchanger networks designed via algorithmic synthesis procedures. For example, the Su algorithm was incorporated in modified form in the RESHEX software from Caltech.

- Finally, Rudy is the father of one of the first flowsheeting programs (CHESS) whose structure has been incorporated in commercial software marketed to the present day."

Jeffrey Siirola Wins the 1991 Computing Practice Award



As "a recognized leader in the area of process synthesis and a respected member of the CAST community," Jeffrey J. Siirola, Senior Research Associate at Eastman Chemical Company in Kingsport, Tennessee, will be presented the 1991 CAST Division Computing Practice Award at the CAST Division Dinner on November 19 in Los Angeles. The Computing Practice Award, sponsored by Pergamon Press, honors an outstanding effort that has resulted in a specific emobodiment, or possibly an industrial or commercial application, of computing and systems technology. The award consists of $1000 and a plaque.

According to the nomination statement:

"Jeff has been personally involved in the practice and application of computing in chemical engineering starting with the AIDES program for the automated synthesis of chemical plants developed during his graduate work. In his early years with Eastman Chemical, he developed computer systems for heat exchanger network design as well as the design of heat-integrated distillation systems. These programs were used to the company's advantage in a number of processes. More recently, Jeff has become involved with the development of hybrid algorithms for the synthesis of entire chemical plants, including distillation system sequencing. He is also involved in the use of advanced computer graphics to provide visual aids to the process designer in determining favorable regions for a process design."

"Jeff has also had a great influence on the engineers with whom he has worked and supervised. In order to more quickly implement design and synthesis ideology, many techniques have been developed to use existing computer software for the task. Some examples are successive simulation to evaluate process flowsheet alternatives, development of specific models (such as reactive distillation) to evaluate new ideas, and the use of simulator thermodynamic packages to produce approximate residue curve maps for distillation column sequencing. Engineers under Jeff's supervision have also been instrumental in developing expertise in the interpretation of simulator results (both converged and nonconverged) to explain and predict operating behavior of existing plants. Some examples of implemented successes with Eastman Chemical are the Chemicals from Coal Complex, the patented process for the production of diethoxy methane, and the understanding of azeotropic distillation facilities for the separation of acetic acid and water."

"He was the first to recognize the application of the then emerging field of artificial intelligence (AI) to chemical plant design. As a pioneer, Dr. Siirola showed the persistence to overcome skepticism among faculty and the NSF bureaucracy to win funding for his pioneering research. The result of his work was a set of computer programs that demonstrated the feasibility of using AI for the design of chemical plants. The seed planted by this work is now bearing fruit at a half dozen universities, and represents the most dynamic part of the current chemical engineering research scene. The work is also incorporated in a book which Dr. Siirola coauthored with his adviser, Dale Rudd, and a fellow student, Gary Powers, and which is now used as a university text."

A supporting letter provided the following comments:

"Jeff Siirola is an outstanding candidate fulfilling the spirit and the letter of the Computing Practice Award for the following reasons:"

"1. His pioneering work on AIDES has made a very long-standing contribution to the area of systems technology by: (i) defining an area of research which still pursues AIDES initial goals, (ii) proposing a systematic methodological approach—the central elements of which can still be found in today's works—that has provided a concise model of the process synthesis activities, and (iii) recognizing the intellectual scope and the role that an emerging field such as Artificial Intelligence would play in the synthesis of process flowsheets."

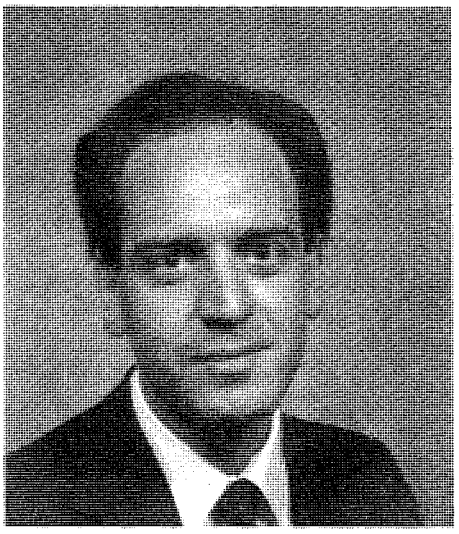
"2. The book on 'Process Synthesis' he co-authored with Rudd and Powers is one of the most imaginative contributions to the chemical engineering literature. It introduces at a very early stage of undergraduate chemical engineering education: (i) the need to be 'creative,' (ii) the rational for the analytical subjects of the chemical engineering science core (to follow), and (iii) offers a first paradigm on how to approach design in a methodological manner."

"3. His industrial practice of the process synthesis methodologies over the last 20 years has endowed Eastman Chemical with improved processes, novel and patentable processes, and simpler and more efficient processes. He has made significant contributions by: (i) reducing energy consumption of several processes through the synthesis of innovative energy integration systems; (ii) reconfiguring the separation sequences of many processes, leading to simpler, less costly and more efficient systems; and (iii) establishing patentable new processing schemes for specialty chemicals."

"Jeff Siirola is an excellent candidate for this Award, not only for the above specific technical contributions, but also for the global impact that he as a person and colleague has had on the practice of computing and systems technology in chemical engineering. More specifically, as trustee and as president of CACHE he has played a pivotal role in formulating the scope and advancing the role of computers/computing/systems technology in chemical engineering education. As a member and officer of the CAST Division he has been instrumental in the continuing vitality and growth of CAST, as well as its impact on our profession. As an industrial research he has had an important impact in shaping academic research in process synthesis."

Dr. Siirola received his Ph.D. from the University of Wisconsin in 1970. He is an industrial trustee and Vice-President of CACHE Corporation. He was the conference chairman for FOPCAPD '89, is a member of the ACS, American Association for Artificial Intelligence, and AIChE; is past chairman of the CAST Division of AIChE; and is currently chairman of the CAST Division Programming Board.

Michael Mavrouniotis is the 1991 Ted Petersen Student Paper Award Winner



The Ted Petersen Student Paper Award is given "to recognize an outstanding published work, performed by a student, in the application of computing and systems technology to chemical engineering." This award, co-sponsored by IBM and ChemShare, consists of $500 and a plaque. The award will be presented at the CAST Division Award banquet at the AIChE meeting in Los Angeles.

The Ted Petersen Award winner for 1991 is Michael Mavrouniotis, who received his Ph.D. from MIT in 1988 and is currently an assistant professor at the University of Maryland. The paper for which Michael was nominated was "Computer-Aided Synthesis of Biochemical Pathways," which appeared in Biotechnology and Bioengineering and was coauthored by George Stephanopoulos and Greg Stephanopoulos. "Michael was the

primary and fundamental originator, designer, and implementor of the work reported in this paper... and deserves the full credit..."

The nomination letter provided the following identification "for a paper which is an important and lasting contribution in the areas of systems theory, computer-aided technology, and biotechnology:"

A. Systems Theory. The paper describes an algorithm for the systematic synthesis of enzymatic pathways satisfying a series of constraints. A. W. Westerberg from Carnegie-Mellon University characterizes this algorithm as "certainly very clever," and "it can find pathways that a previous algorithm by Bailey and co-workers cannot, and it generates the pathways without all the redundant effort of this earlier work." "It is an algorithm based on very sound principles," and "is able to handle significantly larger problems." Jim Davis from Ohio State points out the value of this algorithm from a different angle when he says, "the paper both proposes and demonstrates an elegant approach, which when viewed generically offers considerable insight into general problem-solving synthesis." Indeed, Michael's algorithm can be used for the synthesis of other types of reactions, and in an upcoming publication he will report on the application of this algorithm to the synthesis of catalytic reaction mechanisms. Furthermore, the paper reports on the meticulous analysis that Michael carried out in establishing the properties of the algorithm. Through this logically rigorous analysis he was able to establish theoretically the strengths and weaknesses of the algorithm.

B. Computer-Aided Technology. The synthesis algorithm, discussed above, is the center-piece of Michael's work, but does not stand in isolation. On the contrary, it is organically related with a series of analytical and synthetic tools that Michael developed in order to carry out systematically "Computer-Aided Synthesis of Metabolic Pathways." In reflecting on the scope of Michael's work, Professor Gene Brown, Dean of Science at MIT and a well- known expert in biochemistry, notes: "Initially I was dubious about his thesis project. I thought the scope was too great and the project was too ambitious for a graduate student. He fooled me." Also, as Dr. Liebman, an expert in metabolic engineering from Amoco Technology Company, indicates: "this paper contributes technology for performing computer-aided design/prediction/evaluation." Further on he comments that the essential knowledge representation schemas that Michael developed for the synthesis of enzymatic pathways "will be essential within the Human Genome Project, even beyond the needs of biochemical/biotechnological system analysis." In this regard, Michael's work transgresses the boundaries of the domain for which it was developed, i.e., biochemistry/ biotechnology, and takes a more generic value applicable across different domains. Finally, A. W. Westerberg points out that Michael's research activities have produced a number of other significant contributions—e.g., (a) order-of-magnitude computations, (b) estimation of equilibrium constants for biochemical reactions from group contribution estimation techniques, (c) computation of maximum enzymatic rates, and (d) identification of enzymatic regulation structures—that are compliments of his synthesis algorithm and have all been organically integrated in a computer-aided system called BioPath.

"*C. Biotechnology.* Professor Brown's comments indicate that Michael's work is "an outstanding contribution to the discipline of biotechnology," and that he expects "the work presented in the paper will be used as a model by many investigators interested in maximizing synthesis of various products in multi-enzyme systems." Dr. Liebman, by utilizing the results of this paper already is revealing some of the large impact areas that can benefit from Michael's work. He goes even further to state that "the questions which exist in utilizing/ optimizing/modifying/designing biochemical pathways for use in producing speciality chemicals, reducing side effects and/or toxicity, optimizing yields, tracing evolution relationships in biology, predicting therapeutic target sites and even predicting the impact of genetic variation or defects are examples of the areas which I believe will be positively and significantly impacted upon by his work."

Articles

Chemical Process Synthesis, Design, and Operations Using Supercomputers

by Stephen E. Zitney and Richard D. LaRoche, Cray Research, Inc., 655-E Lone Oak Drive, Eagan, MN 55121

Abstract

Large-scale computations using supercomputers offer new opportunities for efficiently simulating complex chemical processes. Until recently, there has been no significant effort made to develop or optimize application codes for chemical process engineering on supercomputers. However, initiatives at Cray Research, along with leading chemical companies, software vendors, and academic research groups, are signaling an end to this trend. Process engineering tools currently being tailored to run on supercomputers will be discussed with the focus on the center of this application area, the process simulator.

The development of sequential-modular process simulators for use on supercomputers will be outlined along with plans involving equation-based methods for solving chemical process simulation problems. Research efforts in this area involve the development of new strategies for exploiting vector and parallel architectures in solving process flowsheeting problems.

Other initiatives are aimed at integrating process simulation on supercomputers with flowsheet synthesis and plant operations. With the development of more powerful mathematical programming techniques, combined with increasing supercomputer power, it is becoming feasible to rigorously model, optimize, and automate the synthesis process. As network supercomputing makes it possible, the use of supercomputer simulations in a plant operations environment will help to maximize performance around economic, safety, environmental, and regulatory constraints.

1. Introduction

The chemical processing industries face many challenges in the 1990s. Commodity chemical manufacturers are encountering a tight marketplace worldwide and are under constant pressure to maximize production while minimizing waste. Speciality chemical producers are aggressively competing for new market segments, where responsiveness to customers and the ability to customize products are essential. Petroleum companies and natural gas producers are faced with increasing demand and tighter environmental regulations. All companies in the processing industries are trying to improve product quality while lowering production costs.

To meet these challenges and compete successfully in today's global marketplace, more and more companies in the chemical process industries are making the strategic decision to implement supercomputing as an integrated part of their process engineering activities. Processing companies recognize that using supercomputers for process engineering can ensure maximum return on investment by saving capital, materials, operating costs, manpower, energy, and time.

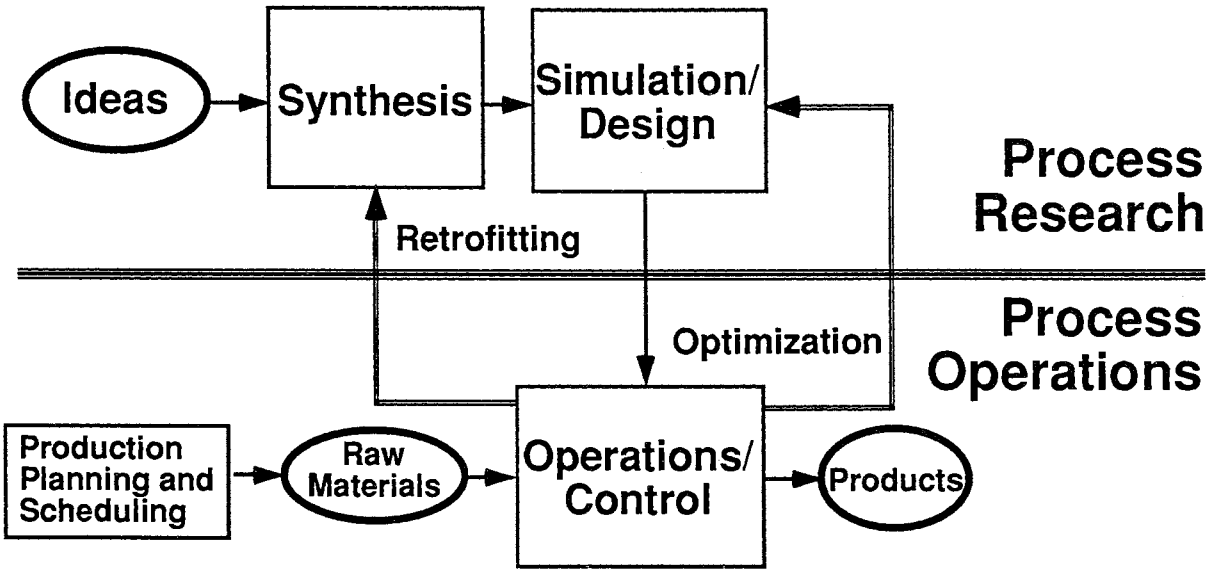


Figure 1. Chemical Process Engineering Activities

Over the past two years, Cray Research has been pursuing an applications-driven program to address the various fundamental process engineering activities shown in Figure 1. We have focused initially on the essence of process research, solving large-scale chemical process simulation and design problems. Early activities (Zitney et al., 1990) have centered on porting and improving the performance of industry-standard process simulators, like ASPEN PLUS, PROCESS, and its successor, PRO/II. This paper will assess the current status of these and other sequential-modular simulators on supercomputers.

The scope of our effort in process research has been extended recently to include process synthesis. This was achieved with the launching of a joint project with Air Products and Chemicals, Aspen Technology, and the Engineering Design Research Center (EDRC) at Carnegie-Mellon University. The objective of this project is to create prototype software which integrates the synthesis and simulation of chemical processes in a supercomputing environment. The scope of the project will be outlined here along with analysis of the opportunities which can be gained by combining supercomputer power with mixed-integer nonlinear programming techniques for the synthesis and retrofitting of process engineering systems.

Large-scale simulation has been most heavily utilized in process research (synthesis, simulation, design, and retrofitting of processing facilities) and to a lesser extent in day-to-day process operations. As network supercomputing environments make it possible, however, we expect increasing demand for the use of full process simulation models in plant operations. By using proven design models on supercomputers to advise in process operation, plants may be operated on the "edge" to achieve optimal efficiency. We consider here the challenges and opportunities involved in developing an integrated high-performance simulation environment for process operations.

2. Process Design and Simulation

The chemical process design and simulation problem entails the solution of a large equation system representing the continuous flow of materials and energy through a single process unit, a network of several process units, or an entire plant site. Typically these simulation models are large systems of nonlinear algebraic equations, but some ordinary and partial differential equations may be included in the system for dynamic simulations.

The computer capabilities required to solve these problems vary significantly depending on the level of scientific detail embedded in the model. Model complexity can range from simple linear representations to rigorous models of the chemical and physical phenomena occurring in the process. Introduction of dynamic modeling or optimization can place additional requirements on computer hardware. In the case of dynamic simulation, the computational requirements increase in proportion to the number of time steps. Optimization problems must be solved iteratively, so their solution time grows in proportion to the number of optimization iterations. The total work required depends largely on the complexity of the objective function, the number of decision variables, and the number and type of constraints associated with the optimization problem. For a given problem type, the computational requirements may also increase in proportion to the number of variables (e.g. components).

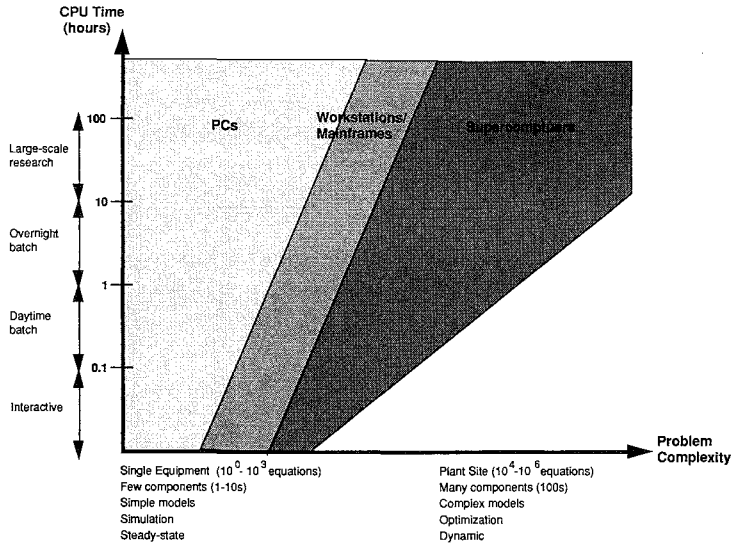


Figure 2. Computational Requirements in Chemical Process Simulation

Figure 2 provides a rough estimate of the computational effort required to solve a wide variety of process simulation problems using computers ranging from PCs and workstations through supercomputers. The shallower slope of the supercomputer line accounts for efficiency gains that arise from taking advantage of vectorization and parallelism. As indicated in the figure, PCs can handle simple steady-state problems interactively and as reasonable batch jobs. But, large-scale optimization or dynamic simulation problems are inaccessible to PCs, which generally execute process simulation codes at speeds well under 1 million floating-point operations per second (MFLOPS). Powerful workstations and mainframes can achieve rates up to several MFLOPS when running process simulation software. For single equipment or small groups of units, these computers can solve complex optimization and dynamic simulations, but only as time-consuming batch jobs. Using the sequential algorithms found in traditional process simulators, supercomputers typically provide at most an order of magnitude performance improvement over mainframe computers (see Table 1). This speedup, due mainly to a faster clock speed, is quite impressive. However, only process simulation software that is designed to exploit the vector and parallel architectures of supercomputers can achieve rates of several hundred MFLOPS—the rates needed for not only the interactive simulation of several complex plant units, but also for the rigorous optimization of an entire plant site.

Over the past two years, considerable effort has been made to port, optimize, and enhance the industry-standard process simulation codes for use on CRAY supercomputer systems (Zitney et al., 1990). Cray Research's research and development program in this area has accelerated in response to a growing interest from processing companies in the chemical and petroleum industries. An update on the current status of ASPEN PLUS, PROCESS, and PRO/II and a look at future activities involving the use of these process simulators on supercomputers is given in the Appendix.

Along with Cray Research's ongoing program to develop and optimize process engineering software for supercomputers, several researchers in the government, academic, and industrial sectors have undertaken some of the initial efforts to assess process simulator performance on advanced architectures. The Los Alamos National Laboratory assessed the ASPEN program on their CRAY-1 system for use in the study of fossil fuel conversion processes, nuclear fuel cycle, and nuclear waste processes (Duerre and Bumb, 1981). A DuPont study (Haley and Sarma, 1989) demonstrated the benefits of using a supercomputer to solve the complex simulations and the day-to-day problems faced by a chemical processing company. Affiliated with the University of South Alabama, Harrison (1989) recently conducted a FLOWTRAN study on the CRAY X-MP system at the Alabama Supercomputer Center.

Table 1 shows that chemical process simulation is a relatively new application area for supercomputers. Most documented studies of process simulators running on supercomputers have appeared in the last several years. Only the report by Duerre and Bumb (1981) on the public

Table 1. Modular Process Simulators on Supercomputers

Process Simulator	Conventional Computer	Supercomputer System	Simulator Speedup			LINPACK[5] Speedup
			Avg.	Min.	Max.	
ASPEN[1]	IBM 370	CRAY-1	2.8	2.0	3.9	55
CPES[2]	DEC VAX 8800	CRAY X-MP	5.5	5.0	6.0	71
PROCESS[2]	DEC VAX 8800	CRAY X-MP	10.5	1.9	67.9	71
FLOWTRAN[3]	IBM 4341-2	CRAY X-MP	6.2	3.5	26.0	368
ASPEN PLUS[4]	DEC VAX 8530	CRAY Y-MP	14.3	11.3	32.6	123

[1] Duerre and Bumb (1981)
[2] Haley and Sarma (1989)
[3] Harrison (1989)
[4] Zitney (1991)
[5] Dongarra (1990) – The LINPACK speedup is the ratio of LINPACK timings (100 x 100 dense linear system) for the supercomputer (1- cpu) over the conventional computer.

version of ASPEN appeared in the literature prior to 1989.

Using the LINPACK speedups in Table 1 as a measure of potential performance improvement, it is clear that the process simulators take little advantage of vector processing. The average simulator speedups, ranging from 2.8 to 14.3, are an order of magnitude less than the LINPACK speedups (55 to 368). Some vectorization occurs in the simulators, but not enough to make a truly significant impact. The overall performance is degraded by the widespread use of scalar coding techniques and sequential algorithms. Fortunately, the performance of these traditional sequential-modular codes can be improved through selective code modification and algorithm reformulation.

Guidelines for developing and optimizing process simulators for supercomputers have been presented recently by Zitney (1991). The development process consists of three key phases: performance analysis, standard code optimization, and algorithm reformulation.

Performance Analysis – Code performance tools are used to identify the most computationally intensive routines in the process simulator. The tools also provide valuable information on the conditions inhibiting vectorization of DO-loops. A large number of representative simulation problems are required for a meaningful analysis. In our experiences with the traditional sequential-modular simulators, namely ASPEN PLUS, PROCESS, and PRO/II, most of the computation time tends to be spent in low-level thermodynamic routines and linear equation solving routines.

Code Optimization – Portions of the simulation code are rewritten to remove conditions that inhibit DO-loop vectorization and to improve the execution rates of vectorizable loops. Optimization examples of this type include inverting loops to avoid a recurrence, segmenting a nonvectorizing loop into multiple loops to minimize the effect of a dependency, and horizontal loop unrolling to reduce number of memory references. Another common approach in this stage of optimization is to use of highly efficient, linear algebra computational kernels (e.g. BLAS) that are designed to include the machine dependent features needed to achieve high performance. While the time savings from standard code optimization can be impressive, the potential for dramatic reductions is usually quite limited and in most cases less than a factor of 10 (Zitney, 1991). A large impact can be made only by reformulating the sequential algorithms in these codes to take advantage of the architectural properties of vector and parallel computers.

Algorithm Reformulation – The routines based on sequential algorithms are redesigned and replaced with the equivalent highly tuned modules for advanced architectures. Algorithms selected for reformulation should not only be used in multiple simulation codes, but also represent a major portion of the total problem computation time. For example, most general-purpose direct linear solution routines found in process simulators are good candidates for algorithm reformulation. Their use of indirect addressing can drastically degrade vector performance. In a recent study, Zitney (1990) demonstrated the impact of redesigning solution algorithms by replacing the traditional sparse MA28 solver in ASPEN PLUS with a frontal code designed for advanced architecture computers. Results on four large-scale distillation problems showed that by avoiding the indirect addressing problem and operating on full matrices, a frontal code can reduce linear solution times on supercomputers by several orders of magnitude. In fact, a single processor of a CRAY Y-MP system using the frontal code ran nearly 250 times faster than a VAX 8530 using the MA28 routine to solve one of the large reactive distillation problems in the study.

As described above, significant performance enhancements for sequential-modular codes can be achieved by redesigning the equation solving routines involved in multistage separation calculations. In view of this opportunity, Cray Research is investigating equation-based methods for solving entire chemical process simulation problems. The equation-based methods differ from traditional modular simulators in that they do not proceed sequentially from process unit to process unit in arriving at a final solution but instead treat the entire chemical process as one large equation set that is solved simultaneously. This approach allows for the efficient solution of problems involving dynamic behavior such as startup and shutdown studies, control and operability studies, and operator training. Most importantly, the equation-based approach to process flowsheeting appears to be very amenable to the vector and parallel processing features of state-of-the-art supercomputers.

In 1991, a joint collaboration between Cray Research and the Institut fur Systemdynamik und Regelungstechnik at the University of Stuttgart in Germany was undertaken to demonstrate the capabilities of equation-based dynamic process simulation on supercomputers using the DIVA program. Cray Research is also exploring opportunities for having other dynamic process simulators available on CRAY systems.

3. Merging Process Synthesis and Simulation

Process synthesis can be viewed as the thinking process by which the design engineer arrives at a flowsheet configuration capable of transforming reactants into the desired products. Once one or several flowsheet configurations are determined, work can proceed with process simulation packages to set design parameters for a workable and hopefully optimal plant design. In merging these two distinct methodologies, the power of process simulation can be used to help guide the oftentimes difficult process synthesis stage. Such an approach presents the opportunity to identify both the optimal configuration and process operating parameters in a single, efficient design methodology.

Merging traditional process simulation with process synthesis requires the ability to handle both continuous and discrete decisions. Continuous design decisions, such as setting equipment operating conditions, are handled effectively with commercially available process simulation systems and nonlinear programming (NLP) software. Process synthesis invariably requires many discrete decisions such as the type and number of unit operations, feed tray locations, and number of distillation stages. These discrete decisions present an integer component which makes the overall synthesis/simulation optimization problem a mixed integer nonlinear programming (MINLP) problem. The MINLP approach involves solving an alternating sequence of NLP problems and mixed integer linear programming (MILP) problems.

Researchers at the Engineering Design Research Center (Carnegie Mellon University) and other institutions have demonstrated the concept of using MINLP techniques to solve problems involving both discrete and continuous design decisions. Grossmann (1990) provides a general overview of the MINLP approach to chemical process synthesis and design. Listed below are some design and operations applications where MINLP techniques can be employed.

Design Examples:

- selection of optimal process flowsheet structures
- synthesis of heat exchanger networks
- selection of feed tray location and number of plates in distillation columns
- retrofits of distillation sequences
- retrofits of steam and power plants
- design of multiproduct batch plants

Operations Examples:

- plants requiring startup/shutdown of units because of demand fluctuations
- plants requiring startup/shutdown of units because of feedstock fluctuations
- multiproduct batch plant operation
- operation of steam and power generation plants with chemical process facilities

Presently, no MINLP capability exists to tackle large-scale industrial problems even though the concepts have been clearly demonstrated by academic researchers (Diwekar, 1990). We are faced with another glaring case of ineffective "technology transfer" largely because the MINLP approach requires a giant leap from traditional design practices. In addition, the computationally intensive nature of MINLP optimization signals that advanced computer architectures employing parallelism will need to be used effectively to make this technology a reality for large-scale industrial process engineering.

The next step toward translating these techniques to industrial practice is to integrate MINLP capabilities in a framework where commercial simulators can be used to solve industrial problems. Such a mission requires effective integration of computer software, computer hardware, algorithm development, and industrial applications which is practically impossible for any single organization. In 1991, the following project team was formed to create a prototype system integrating the synthesis and simulation of chemical process plants using MINLP techniques and to demonstrate its capabilities by solving realistic industrial problems.

- Air Products and Chemicals
  industrial applications and experience
- Aspen Technology, Inc.
  flowsheet software vendor (ASPEN PLUS)
- Cray Research, Inc.
  supercomputer vendor (CRAY Y-MP)
- EDRC
  algorithm research and development

4. Merging Process Operations and Simulation

Many processes in operation today were designed or retrofitted with the help of rigorous process models from in-house or commercial simulation packages. These same proven models can be used to maximize the performance of current plant operations around economic, environmental, and safety considerations. The use of design models by plant operators can then in turn supply valuable information on how to improve future designs. Such an approach offers the opportunity for consistency and continuity throughout the entire life-cycle of a project from process development through to plant operations. Listed below are some

plant operation activities that would benefit from the use of rigorous process models.

- startup/shutdown guidance
- rate/grade transition for feedstocks and products
- process monitoring
- equipment maintenance and fault detection
- operator and engineer training
- process optimization
- advisory process control
- production planning and scheduling
- safety and environmental evaluations

Merging traditional process simulation with plant operations provides the capability to use rigorous models off-line as prediction tools or on-line to help run the plant more efficiently. In an off-line mode, process simulations can be used to perform "what if" studies in which operational strategies are tested without ever actually changing the operating process. This presents the opportunity to predict the effect of process disturbances and fluctuating economic conditions on overall plant performance. In an on-line capacity, full process models can be run on a computer using current process conditions to advise on plant operation. On-line simulation results can be used either as a guide to plant operators, or directly to provide set points to the distributed control system in the plant.

For on-line modeling, the issue of efficiency is critical. A process engineer needs the results of the simulation before operating conditions change. As a result, early industrial applications of on-line modeling were based on simple models of the plant coupled to nonlinear programming codes. Even today, it is not practical to solve rigorous on-line models on conventional computers. Only supercomputers offer the opportunity to efficiently use full process simulation models in connection with plant operations. A network supercomputing environment for plant operations will allow on-line applications to be distributed within the plant network. Other systems on the network perform data handling, graphic display, and other functions, while the supercomputer handles the rigorous process simulations.

Inevitably, rigorous simulations used in plant operations will be based on dynamic models, and increasingly aspects of dynamic behavior will be incorporated throughout the whole design process. This is because a plant rarely runs at steady-state owing to a wide range of disturbances. Dynamic simulation systems provide moving snapshots of a process in action. These systems calculate the transient behavior of a plant over time using differential algebraic equations, but require an enormous amount of computational effort for solving industrial scale problems. Executing these full process dynamic simulations is only practical with the use of powerful supercomputers.

Cray Research is engaged in the development of a prototype computer-integrated, model-based simulation environment for process operations. Such an environment is critically dependent on the effective integration of the following:

- robust, flexible, and efficient process simulation software
- accurate plant models
- consistent, reliable and accurate plant data
- reliable and efficient network communication capabilities
- high-performance plant control and computer systems

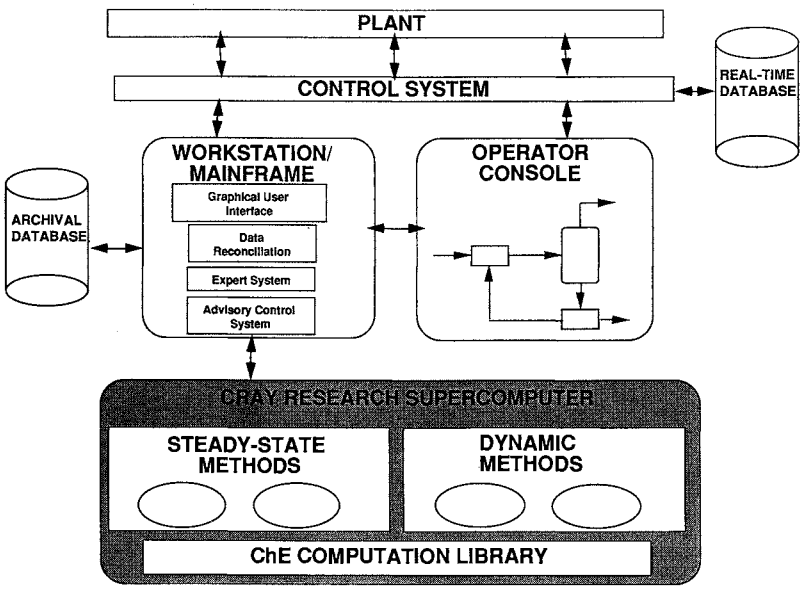


Figure 3. Computer-Integrated Environment for Process Operations

Where possible, activities to develop this environment will be coordinated in partnership with processing companies, software vendors, academic research groups, and providers of plant control systems.

The integrated simulation environment is envisioned to include the following layers of application software and tools (see Figure 3):

- A collection of chemical process simulation codes and MINLP software for modeling steady-state and dynamic processes. These codes will give plant operators and engineers high-performance on vector and parallel computer systems.
- A collection of software tools that allow an operator to interface with the plant, process databases, and the process simulators. These tools fall into the following categories:

  Graphical User Interfaces – interactive interfaces for constructing 2-D flowsheet models on a UNIX-based graphics workstation.

  Intelligent Front-End Software – expert systems and advisory control systems that integrate with the distributed control system and other plant monitoring equipment to access and interpret process data.

  Network Communications and Control Software – software to coordinate message handling and data passing between supercomputer and other network systems.

  Data Reconciliation Software – statistical methods that take real time process data which are subject to random error, bias, as well as gross error and turn it into consistent and reliable input for the simulation.
- A library of highly optimized mathematical routines for chemical process simulators that accelerate performance in a supercomputing environment.

The process simulation packages, MINLP software, and high-performance library will reside on the supercomputer while the system integration software is implemented on one or more mainframes, workstations, or PCs. This model environment reflects the network supercomputing concept developed at Cray Research. In this concept, the supercomputer is seen as a component in a heterogeneous hardware environment, with links between the supercomputer and other mainframes, file servers, and workstations.

5. Concluding Remarks

Chemical processing systems form the backbone of modern industrial production. Continued technological advances for improving the synthesis, design, optimization, and operation of these systems by computational simulations will enhance our ability to solve the complex problems facing the chemical process industry.

Commercial process simulation packages allow the modeling of unit operations at an unprecedented level of detail and accuracy. Supercomputers make it possible to apply these methods to complex processing systems of great industrial importance in chemicals, refining, pulp and paper, and many other application areas. Workstations with powerful graphics provide the capabilities for convenient direct manipulations of the simulated process flowsheets and precise visualization of the calculated results. The stage is set for making large-scale numerical simulations an indispensable tool for all phases of process engineering activity.

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Appendix

Process Simulators on Cray Research Supercomputers: Recent Progress and Future Activities

ASPEN PLUS

ASPEN PLUS 8.2-6 is available on CRAY supercomputers running the UNICOS operating system. The "official" ASPEN PLUS shell scripts can be used for all variations of ASPEN PLUS runs

(edit runs, user databanks, reusable load modules, etc.). On the standard suite of 49 test problems from Aspen Technology, the unoptimized ASPEN PLUS 8.2-6 code was an average of 14 times faster on one processor of a CRAY Y-MP system than on a VAX 8530 mainframe (Zitney, 1990a). Optimization work at Cray Research is well under way on the critical sections of ASPEN PLUS.

Aspen Technology has recently released ASPEN PLUS 8.3 with ModelManager for use on CRAY supercomputers. This latest version has interactive simulation capabilities that allow the engineer to review simulation results, make changes, evaluate process alternatives, and perform case studies rapidly and interactively. Using ModelManager on a workstation or personal computer, engineers can receive expert-system assistance to construct a rigorous flowsheet model. This will enable the use of graphics workstations for the visualization of the flowsheet design process, coupled with the high-speed solution of the process simulation equations on a supercomputer. The result being a network supercomputing environment which increases the abilities of chemical engineers to solve critical chemical process engineering problems.

RATEFRAC, a rate-based nonequilibrium separation process model, is available with ASPEN PLUS 8.3 on Cray Research systems. Engineers can use RATEFRAC to design and develop operating strategies for multicomponent, multistage separation processes such as distillation, absorption, and desorption. The computation times are significantly greater for RATEFRAC than for equilibrium-based models, particularly for problems with a large number of chemical components. On conventional machines, RATEFRAC solution times increase approximately with the square of the number of components, and can be as much as an order of magnitude more than equilibrium-based model times for the same problems. The solution technique employed in RATEFRAC is a Newton-based correction approach that uses the Harwell MA28 routine. The frontal code implemented in ASPEN PLUS by Zitney (1990) appears to offer great promise for solving these very large sparse distillation systems on vector-parallel architecture computers.

An interface between ASPEN PLUS 8.3 and a commercial real-time expert system is being developed at Cray Research to combine rigorous simulation capabilities with rule-based decision-making capabilities. This powerful combination can benefit many off/on-line applications in process operations.

PROCESS and PRO/II

PROCESS 4.01 is available on CRAY supercomputers for both the COS and UNICOS operating systems. Haley and Sarma (1989) reported that a single cpu CRAY X-MP increased performance on an average of 8 to 10 times over the VAX 8800. The minimum ratio of CRAY to VAX performance was 1.9 and the maximum was 67.9. A cost analysis showed that the CRAY X-MP supercomputer was the more cost-effective solution. For DuPont users, the average cost per run on the CRAY X-MP computer is about half as much as on the VAX. It is important to point out here that many of the important PROCESS routines could have run significantly faster if they were optimized or redesigned for vector and multiple cpu operation. However, those involved in the project from DuPont, Cray Research, and Simulation Sciences chose not to pursue this since the follow-up to PROCESS, namely PRO/II, was due out in the near future.

PRO/II incorporates virtually all of the features of its predecessor, PROCESS, in performing rigorous material and energy balances for chemical process flowsheeting applications. PRO/II represents a complete redesign of the flowsheet simulator structure with the goal of integrating the functionality of PROCESS and ASPEN/SP. Currently a pre-release version of PRO/II is running under UNICOS on the CRAY X-MP and CRAY Y-MP. Earlier versions of PRO/II were tailored for the microcomputer environment. PRO/II 3.01, which is due out in 1st Quarter, 1991, is the first version to support computer platforms all the way from PC to supercomputer. Development work to enhance PRO/II's performance on CRAY supercomputers is being done in a collaborative effort between Simulation Sciences and Cray Research. Simulation Sciences has also shown a strong commitment to facilitate the use of PROCESS and PRO/II in chemical process operations with auxiliary packages such as DATACON (for data reconciliation) and ROM (for rigorous on-line modeling).

Object Oriented Programming

by Ron Fosner, Lotus Development Corporation, 1 Rogers Street, Cambridge, MA 02142

You have probably noticed that "object-oriented" is a particularly popular adjective at the moment. But what does it really mean? Many new languages and programs claim to be object oriented, and many old ones have had "object-oriented" ("OO") extensions tacked on, but what does OO mean to the engineer who is responsible for producing a piece of software, and how can they benefit from it?

This article will provide a quick overview of what makes a language object-oriented, and what are the benefits that you can expect from using OO techniques. If you have never programmed in an OO language, you will be surprised. Yes, there are things called "objects" or "classes" or "abstract data types" and they do send "messages" to each other. An "object" is just a collection of data, and (here is the new idea) procedures for manipulating that data. By procedure I mean a subroutine or function. This was a surprise for me when I first started programming in an OO language—finding a piece of structured programming in the bowels of an object—but it makes sense. Just as structured programming brought order by giving us data structures and subroutines, OO programming gives us objects. Objects are simply a way of uniting data and functionality together into a distinct unit.

What makes an Object Oriented Language?

You can get almost as many definitions of an OO programming language as there are languages themselves. But they all tend to involve four basic parts: data abstraction, encapsulation, inheritance, and polymorphism.

Data Abstraction

Data abstraction simply means being able to define your own types of data. In the same manner that you might have integers and floating point data types, data abstraction lets you create a new type of data complete with its own unique methods for observation and manipulation. This is the seed of the famous "object" or "class" of OO programming.

Some FORTRAN programers make extensive use of the complex data type. Adding two complex numbers simply means using the addition sign in a statement. In the OO language C++, programmers have this same option, even though C++ does not have a complex data type built in. C++ is an extension of C, and starts off with the same core data types. But most C++ environments come with a complex number library in which the functionality of the FORTRAN complex data type is duplicated.

C++ is a language that also supports something called operator overloading, meaning that the creator of an object in C++ can describe how, for example, the plus sign operates when told to add two numbers if one or both is a complex number. The same capability can be given to vector and matrices. I have some programs that manipulate matrices, and it is much simpler to understand (and write) "A+B" than "call matrix_add(A,B)." Operator overloading is a supplement to data abstraction, and is not supported by all OO languages.

Encapsulation

The whole philosophy of OO programming is one of a client-supplier relationship. This becomes most evident in the ability of OO languages of encapsulation. Once you, as the supplier, have created an abstract data type for use by "clients" (i.e., everyone who uses your data type), you also provide public access to parts of the data type.

Encapsulation means that the private data and the methods of manipulating that data are the property of the class, and that the client cannot access data or methods that are not explicitly made public. Thus, your class becomes much like a built-in data type; you are not granted access to machine code floating point routines, and you probably really do not want to be. Encapsulation ensures that you cannot, even unintentionally, trash information that you are not supposed to have access to. This has the effect of isolating problems since everything about a class in encapsulated in the class. Problems usually become easily identified and located.

Inheritance

Inheritance refers to the ability of one object to inherit the operations and information of another object, usually with the intention of extending and specializing these items in the new object. Some languages support multiple inheritance, which is simply inheriting the abilities from one or more parent objects.

When you need to create an object that behaves almost, but not quite, the same as an existing (and we can assume, already debugged!) object, inheritance is the answer. You simply create the new object as being derived from the object it principally resembles, and just add the parts that you need. You are then left with the job of testing only those parts that are new. The added benefit is that all the methods that were inherited usually stay with the parent object; in other words, those methods that operate exactly the same as the parent object actually use the same, debugged code as the parent object.

An example is deriving a vector object from a matrix object. A vector is just a special case of a matrix. Vector multiplication is just the same as matrix multiplication, and thus could use the same methods, but you might want to add a new method for computing the dot product of a vector.

Inheritance also promotes efficiency. If a object is modified to be more efficient in some manner, or a bug is fixed, or new capabilities are added, then all objects that inherit from this object inherit the change.

Polymorphism

Polymorphism is the ability for one of the methods of an object to be redefined in a derived object. In the vector-derived-from-a-matrix example given above, you certainly could use the matrix method of multiplying a vector, but you would significantly improve execution speed by rewriting the routine specifically for vectors. Thus, multiplication becomes polymorphic—multiple procedures for the same method. It is the job of the language to figure out what you mean, not for you to have to explicitly worry about it.

This also means that you get reusability. If you have an object that almost does what you need, except that one method is not right for this new object, then you simply create a new object that inherits from the almost right object, and modify the functionality that needs change. Everything else that was left remains untouched, and unbroken. Only the new method needs to be tested.

What does being Object Oriented mean?

This is the crux of the matter. Is there really a benefit from being OO? To reflect upon the history of programming for a moment, do you think you benefited from the advent of structured programming? Would you really like to write a program today if you could not use things like subroutines or data structures? Probably not, and I think the impact of OO programming is going to be even more substantial. Structured programming came about when people had to write large programs—programming in the large. OO programming is becoming important as we enter the stage of programming in the huge—that is, programming done by a team of programmers or programs that approach or surpass the 100,000 lines-of-code mark. At this stage it gets complicated veryquickly. Why not let the language take care of the details?

There are many smaller benefits to OO programming, but the two most important benefits that come out of programming in an OO style are reusability and modularity.

Reusability

OO design forces you to think of designing your system as a collection of interacting objects, as opposed to a serial stream of execution. This means that you end up with an assortment of objects with different requirements. From this group you can then select those that resemble objects that already exist in your library, or those that will have to be written from scratch. You will end up with a collection of objects that express various algorithms, interfaces, data structures, or tools.

Unless this is the first program you have written, and you have no existing library or code to access, you will probably be able to get from 20 to 70% of your objects from existing sources. I have found that, particularly as I increasingly write code for other peoples' consumption, the user interface typically accounts for 40% of my finished product. Not only does my productivity increase as I reuse objects, the code is more robust since these objects have already been tested.

Modularity

Modularity is the encapsulation of behavior into an object or group of objects. Modularity is a natural effect of OO design. Procedures and data tend to get collected into "chunks" of code that make up an object or object group. This promotes reusability as well as robustness. Debugging an object that has a very explicitly described and expected behavior is a much simpler process than debugging a large subroutine, which either works or does not work. I once had to add a help system to a program that I was working on. Looking around the company, I found one that did what I needed and was fairly modularly designed. I had to hook in my input and display routines, but after four hours of work, I had a fully functioning help system that never had any bugs reported on it. This was not an OO program, just a straight C program, but you can see the benefits from having reusable modules. If you can routinely get even 30% of your code from an existing library, and not have to worry about testing that 30%, you will realize a significant savings in time and effort.

Creation of Objects for Unit Operations

OO design is a design of building blocks. Rudimentary objects are created that encompass the basic behavior of one or more elements, and these are, in turn, used to create more complex objects. This process continues until an object is created that mimics one of the elements of the programming project. For this paper, I decided to attempt to design prototype objects for a rudimentary unit operations collection.

One of the basic questions that people ask about OO design is "How do you decide what makes up an object?" The

answer is that you will not know if you did it right until the objects have had a chance to mature. Mature objects are the ones that get used most frequently, are simple enough that they are useful when inherited, but complex enough to provide significant features, and those that successfully encapsulate some "feature" that is analogous throughout the program for which you are designing the object. In other words, after you have designed and written the objects, if the final program is simply a matter of connecting objects up to each other, the design worked. If you find that you need to tweak each object one way, then another, for each occurrence, then the design was bad. Designing objects has been compared to designing integrated circuits—to assemble a computer, you get the chips that do the jobs you need and wire them together. Objects are the "chips" of software.

I still have not answered the question of how to decide what makes up an object. There is no single correct answer, since more than one design can be successful. One useful suggestion is to write a description of what you are trying to do in detail, then collect the nouns. This is a good starting point for deciding what can be a successful object. A useful object is one in which the behavior is intuitive, and this is easiest to accomplish when the object mimics some concept or physical object. For unit operations, one of the basic capabilities needed is the simple transport of chemicals. It is a feature used in all aspects of unit operations, and is one that is easy to conceptualize. You may be surprised at how "granular" my first object is, but as you will see, it provides an excellent building block for all other unit operations.

The "PORTAL" object is my basic building block for describing chemical transport. A PORTAL object is the transport mechanism through which chemical components pass from or through a unit operation module. The structure of a PORTAL object (in pseudocode) is shown below.

```
PORTAL {
   variables
   temperature, pressure, composition

   procedures
   print variables
}
```

All objects have a data area and a procedures area. The PORTAL object is what is called an abstract object. There is no concise physical metaphor for a PORTAL. It models that aspect of a unit operation involved in the transport of a chemicals stream from one physical location to another. It is easier to use than explain.

A PORTAL has three variables: temperature, pressure, and something called composition, which encompasses chemical composition, vapor fraction, etc. A PORTAL also has just one procedure, the ability to print out the variables to some unspecified device.

A simple application of a PORTAL is to describe a pipe. A pipe is just two portals separated by some distance, with a corresponding pressure loss. The PIPE object can be created by the following declaration;

```
PIPE {
   variables
   PORTAL *inlet, outlet   ; A pipe has
                             two Portals
                             in it
   length                  ; and a length

   procedures
   calculate output composition and
   pressure loss
}
```

I have used the asterisk of C and C++ notation to indicate that the inlet PORTAL is a pointer; that is, the PIPE object can reference the inlet PORTAL, but does not own it, it belongs to some other object. This design implies that a unit operation can only modify its own outlet conditions, not its inlet. In addition, the PIPE object uses the length variable to calculate the pressure drop and thus modifies the pressure variable in its outlet PORTAL. The PORTAL objects that make up the PIPE object still contain their variables and procedure; a PIPE can request that each PORTAL print out its variables.

A generic unit operations object can be created from a collection of PORTAL objects, plus some method (i.e., a subroutine) for changing the variables of the outlet PORTALS. In fact, this is a good description of a unit operation: one or more inputs are subjected to some (unspecified) process, resulting in one or more outputs.

```
UNIT_OP {
   variables
   PORTAL *inlets[], outlets[]

   procedures (VIRTUAL)
   calculate output compositions,
            heat and pressure changes,
            material balance
}
```

The brackets after inlets and outlets indicate that there is one or more of these objects; in other words, these are arrays of PORTALS. The asterisk again indicates the array comes from outside the object. The one procedure for the generic UNIT_OP object has the preface VIRTUAL. This is a useful property which indicates that the UNIT_OP object is nothing more than a template; a virtual procedure is one that is expected to be replaced when a new object is created that inherits from the UNIT_OP object. The new procedure will have to specify exactly what the procedure does.

The UNIT_OP object provides a template for our first "real" object—a tray in a distillation column. An idealized tray consists of an inlet vapor stream, an outlet vapor stream and inlet liquid stream, and an outlet liquid stream.

```
TRAY <UNIT_OP> {                          ; we inherit everything that is
                                          ; in a UNIT_OP object
    variables
    outlets[2]      ; specify # of outlets
    *inlets[]                             ; inlets specified elsewhere

    procedures                            ; define the VIRTUAL procedure
    calculate output compositions,
                heat and pressure changes,
                material balance
}
```

While this is a simple example, it is not far from what an actual program might look like. Admittedly, in the procedure of the TRAY object, there is quite a lot going on. But that complexity is hidden from users of the TRAY object. The procedure itself would be built up from similarly constructed building blocks for chemical separation. Each tray "knows" how to modify the outlet composition by calling on a thermodynamics package, and performs a material and heat balance. The inlets of the tray are specified elsewhere, typically coming from another TRAY object. We also need a CONDENSER object, a REBOILER object, and a FEED_TRAY object to complete our distillation column.

I make no claim that this is an efficient structure. On the contrary, this example is simply intended to be an illustration of how these objects can be constructed into a whole entity in order to give you a feel of how an OO design progresses. Realistically one might spend a month or two just trying to decide what the best objects are that model the process. Designing the right set of objects will make the entire program fall together.

The Future of Object Oriented Engineering

While OO programming has been a popular buzzword for the last two years, OO programming has actually been around a lot longer. Simula67 developed the object concept, and most of the more modern OO languages have been built off of the foundations laid by early attempts at what we know of now as OO programming. What we are seeing now is not a flash of enthusiasm based upon a new and sexy concept, but one based upon the development of ideas that have been simmering for the last twenty years.

The biggest challenge that faces anyone interested in learning OO programming is getting used to thinking in OO terms. I have attended seminars and read lots of books, but the best way I have found is to actually attack a problem with an OO tool. You can read and listen all you want, but until you actually learn to think in OO terms, you will not really get any of the benefits.

I have seen no better expression of this idea than in the following quote from an article written by Jim Waldo [1].

"... For about four months I wrote a lot of code. Then, in what I have found is a common occurrence among programmers, I realized that all this code was just C written using C++. It was not object-oriented at all... Management was not happy when it was recommended that four months of work be scrapped... What surprised both the managers and the implementation teams was that doing the work in correct object-oriented fashion proved so efficient that the original production schedule was met. That, too, seems to be a common occurrence among those switching to C++."

Yes, there is definitely a learning curve. However, the benefits do exist, and it is the direction that the software industry is moving towards. One recent article I read stated that within ten years all programming will be done with OO tools and that any programmer who does not know OO methods will be obsolete. In general, I tend to agree with this statement. Chemical engineers tend to think of themselves (justifiably, I think) as being well educated and intelligent, able to adjust quickly to new working conditions and technology. So, if you are not currently using, or experimenting with, or at least evaluating an OO language, you run the risk of missing out on what is going to be an explosive wave of productivity. As more and more people write OO programs, the resources available to programmers, both in terms of object libraries, and development environments, will swell to huge proportions. Now is the time to learn to swim in an OO environment, or sit on the beach and watch all the activity.

Bibliography

[1] Waldo, Jim. "O-O Benefits of Pascal to C++ Conversion", The C++ Report. Vol. 2, No. 8, September 1990.

Suggested Reading

The following is a list of books and periodicals that can get you started in understanding OO methodologies. Unfortunately they tend to represent my bias towards C++, but the periodicals discuss other OO languages as well.

The Tao of Objects, Gary Estminger, 1990, M&T Publishing, Inc., ISBN 1-55851-155-5. A delightful little book that is the best I have seen in trying to give you the flavor of OO design.

Data Abstraction and Object-Oriented Programming in C++, Keith Gorlen, Sanford Orlow, and Perry Plexico. 1990, John Wiley & Sons. ISBN 0-471-92346-X. Gorlen wrote the NIH Class Library for C++, a library that mimics the Smalltalk class library. Some people do not like the "everything is derived from one SUPER object" design, but the book is an excellent discussion on how to design a powerful and generic class library. The NIH Class Library is in the public domain.

Using C++, Bruce Eckel, 1989, Osborn-McGraw Hill, Inc., ISBN 0-07-881522-3. Oriented towards engineers, it is a good, big, book that covers lots of ground. It is spotty in some areas, but Eckel gives lots of examples, and most will find his extensive MATRIX objects useful.

Object-Oriented Software Construction, Bertrand Meyer, 1988, Prentice-Hall Inc., ISBN 0-13-629031-0. Meyer designed the Eiffel language, and this textbook uses Eiffel in its examples. I found it a bit dry, but his production-oriented outlook brings up some important issues.

The C++ Report. P.O. Box 3000, Dept. CPR, Denville, NJ 07834. (212) 972-7055. Published 10 times a year, and containing about 26 pages an issue, it still provides a wealth of very technical issues dealing with using and implementing C++.

Journal of Object-Oriented Programming. P.O. Box 3000, Dept. OOP, Denville, NJ 07834. (212) 972-7055. Published 6 times a year, and about 100 pages, it gives a bit wider. coverage than the C++ Report, but it covers all OO languages. You will find more non- technical articles and more management related ones that in the C++ Report.

Communications

A Monograph Series on Artificial Intelligence in to Process Systems Engineering

by James F. Davis, Ohio State Univ. and George Stephanopoulos, MIT

A series of monographs have been and are being written by the CACHE AI in Engineering Task Force. The monographs are for use as main or supplementary material in advanced undergraduate and graduate courses addressing the application of AI or as a working introduction to AI by practicing engineers.

Three monographs in the series are now available. The purpose of these first three monographs is to provide detailed discussions on the principles, ideas, techniques, methodologies and issues of AI as they apply to chemical engineering. Later monographs will address object-oriented programming, neural reasoning techniques and approaches to specific problems of direct interest to chemical engineers such as fault diagnosis, design, etc.

The monographs currently available are:

Volume I, entitled, "Knowledge-Based Systems in Process Engineering: An Overview," is authored by George Stephanopoulos of MIT. This volume serves as an introduction to the monograph series and provides a broad perspective on AI. Specifically, this volume addresses the scope, history and market of AI and defines the need and role of knowledge-based systems in chemical engineering. Particular attention is paid to describing the general issues surrounding software and hardware environments.

Volume II, entitled, "Rule-Based Expert Systems in Chemical Engineering," is authored by James F. Davis and Murthy S. Gandikota of Ohio State University. This monograph focuses specifically on the implementation of knowledge-based systems in rule-based languages. The emphasis is not on the mechanics of rule-based programming environments, but on the issues which impact the implementation and performance of a system. While the focus is on rule-based implementations, many of the issues discussed cut across all general purpose implementation language. Using specific examples, the monograph covers these issues in detail. As a stand alone chapter, several of the most popular methods for various kinds of uncertainty handling are discussed and compared.

Volume III, entitled, "Knowledge Representation," is authored by Lyle Ungar of the University of Pennsylvania and V. Venkatasubramanian of Purdue University. The content of this monograph is directed at two distinct aspects of knowledge representation. In the first part of the monograph, the problem-independent issues and features of a variety of knowledge representations are presented. Included are discussions on semantic networks, frames, scripts and object-oriented programming. The second part addresses the subject of qualitative physics applied in chemical engineering. The issues of representing structure and behavior are discussed in detail. Examples demonstrating two philosophies are used to illustrate advantages and limitations.

In addition to the monograph series, the task force also has available a series of case studies. The purpose of the case studies to provide the chemical engineering community with detailed examples of the use of AI methodologies to solve chemical engineering problems, a series of three case studies have been published. The three case studies are of sufficient scope to bring out implementation issues, but are small enough for easy understanding. As rule-based implementations, they are complementary to Monograph II described above. These case studies were drawn from projects in an expert system course taught by V. Venkatasubramanian who is presently with Purdue University. Each of the case studies includes:

1. Methods for representing the knowledge,
2. Details on the search methodologies used,
3. Lists of rules and their structural organization,
4. Details on the computer implementation,
5. Alternative scenarios to be explored.

Authored by V. Venkatasubramanian and edited by George Stephanopoulos, the three case studies are as follows:

1. CATDEX: An expert system for troubleshooting a fluidized catalytic cracking unit
2. PASS: A Pump selection expert system
3. CAPS: An Expert System for Plastics Selection

The monographs and case studies are available through CACHE. The monographs are $15 each or $35 for the set of three. The case studies are $17 each or $35 for the set (for sponsoring departments $10 each or $20 for the set).

CACHE Corporation
Attn. Janet Sandy
P.O. Box 7939
Austin, Texas 78713-4933
(512) 471-4933

Cray Research and Prosys Technology Jointly Develop Chemical Process Simulator for Supercomputer Use

by Stephen E. Zitney and Richard D. LaRoche, Cray Research Inc., 6550-E Lone Oak Drive, Eagan Minnesota, 55121-1560

Cray Research, Inc. has signed an agreement with Prosys Technology Ltd. (ProsysTech), of Cambridge, England, to jointly develop a high-performance version of ProsysTech's SPEEDUP software for use on Cray Research supercomputers. Product availability is scheduled for the first quarter of 1992.

SPEEDUP is a software system used to calculate and solve problems associated with chemical process engineering. Based on original research work conducted at London's Imperial College, SPEEDUP has proved to be a dynamic chemical process simulator that can improve quality and yield, reduce operating costs, and enhance the safety and environmental conditions of chemical processing plants. SPEEDUP is used by over 100 major process industry companies around the world.

Using the SPEEDUP system on a Cray Research supercomputer will benefit many industries including chemical, petrochemical, gas processing, oil refining, inorganics, pharmaceuticals, nuclear energy, electric power, minerals, pulp and paper, food processing and waste and water treatment. With SPEEDUP a process engineer can perform the widest spectrum of simulations associated with chemical processing:

- dynamic simulation, design and optimization
- steady-state simulation, design and optimization
- parameter estimation
- data reconciliation

Cray Research and ProsysTech will work jointly to optimize the performance of SPEEDUP on Cray Research systems. The Cray Research version of SPEEDUP will feature substantially enhanced abilities to solve larger, more complex industrial problems for design and chemical process operations.

Chemical plants rarely run at steady-state due to changes in feedstocks, operational objectives and settings, and because many plants are batch or cyclic in operation. SPEEDUP provides a continuous view of a process in action by calculating the transient behavior of a chemical plant over time. Cray Research supercomputers employing parallelism will offer significant advantages to make this technology a reality for large-scale industrial problems.

"Dynamic simulation of entire chemical plant operations is computationally intensive and benefits from the high performance of a supercomputer," said Dr. Peter Winter, market services director for ProsysTech. "Our alliance with Cray Research will enable this technology to provide solutions for the most demanding industrial projects."

As part of the agreement with Prosys Technology, Cray Research is sponsoring a limited number of university licenses for the Cray Research version of SPEEDUP. With this approach, Cray Research and ProsysTech will assist engineering students in gaining experience with equation-based, dynamic simulation methods for chemical processing problems.

"We're proud to be joining forces with ProsysTech to deliver its SPEEDUP product to customers at the high-performance computing level," said Ed Masi, executive vice president of marketing. "Dynamic process simulation is rapidly becoming an important application in the chemical industry. With SPEEDUP on a Cray Research system, engineers can solve the large, complex chemical process problems required to improve plant production and profitability, as well as minimize safety and environmental risks."

Prosys Technology is the leading supplier of chemical process engineering software for dynamic simulation and integrated design.

Cray Research, Inc. designs, manufactures, markets, and supports high-performance computer systems for scientific and engineering applications.

For more information about SPEEDUP on Cray Research computer systems, contact Dr. Peter Winter, Prosys Technology Limited, Sheraton House, Castle Park, Cambridge CB3 0AX, England; telephone: (0223) 312220; or Dr. Stephen E. Zitney, Cray Research, Inc., 655-E Lone Oak Drive, Eagan, MN, 55121; telephone: (612)683-3690; e-mail: sez@cray.com.

Cray Research Makes Available University Licenses for SPEEDUP

by Stephen E. Zitney, Cray Research Inc., 6550-E Lone Oak Drive, Eagan Minnesota, 55121-1560

SPEEDUP is a software system used to solve problems in chemical process engineering. Over 100 major process industry companies and 30 universities around the world are using this software system. Based on original research work conducted at London's Imperial College, SPEEDUP can perform the widest spectrum of simulations:

- dynamic simulation, design and optimization
- steady-state simulation, design and optimization
- parameter estimation
- data reconciliation

Cray Research, Inc. and Prosys Technology Ltd. (ProsysTech), of Cambridge, England, are jointly developing a high-performance version of ProsysTech's SPEEDUP software for use on Cray Research supercomputers. Product availability is scheduled for the first quarter of 1992.

As part of the agreement with ProsysTech, Cray Research is making available a limited number of five-year, educational licenses through the Cray Research University Research & Development Grant Program. Educators and researchers from participating universities can apply for grant funds to cover the cost of the Cray Research version of SPEEDUP. Awards will based on proposed use with priority given to universities that show educational and research use.

A university can be authorized to install and use the SPEEDUP code on a Cray Research system at a national supercomputer center. Each license sponsored by Cray Research permits SPEEDUP to be used only by a single university affiliated with such a center. Accordingly, each university accessing SPEEDUP on a Cray Research system at a supercomputer center must have an academic license for the Cray Research version of SPEEDUP.

SPEEDUP updates are also being handled at a lower cost for these Cray Research sponsored licenses. ProsysTech will provide the updates for a nominal fee intended to cover the cost of distribution of such updates.

With this approach, Cray Research and ProsysTech will assist engineering students in gaining classroom experience with dynamic simulation. The use of SPEEDUP on Cray Research systems will not only improve student productivity, but also serve to encourage R&D projects which further the academic application of supercomputing to chemical engineering problems.

For more information on how to apply for a SPEEDUP academic license on Cray Research systems, please contact:

Stephen E. Zitney
Cray Research, Inc.
655-E Lone Oak Drive
Eagan, MN 55121
Phone: 612-683-3690
E-mail: sez@cray.com

Meetings, Conferences, 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. Siirola (CAST Division Programming Chairman), Research Laboratories – B95, Eastman Chemical Company, PO Box 1972, Kingsport, TN 37662, 615-229-3069, 615-229-4558 (FAX), siirola@kodak.com (email).

Strategic Implementation of On-Line Expert Systems in Process Operations

Columbus Ohio
September 11–12, 1991

A two-day short course aimed specifically at the application of on-line expert systems in process operations. The course will present a practical treatment of knowledge engineering, real-time computing, on-line data interpretation and implementation strategies. Additionally, the course will offer coverage on project justification, planning, and staffing.

Persons involved with any aspect of budgeting, planning, and implementation of on-line advisory systems and intelligent process control systems will find the course useful. The course will provide a focussed coverage of the use of knowledge-based, neural reasoning, and conventional techniques. Specifically, participants will receive information that will enable them to select an on-line expert system application taking into account both business and technical perspectives; determine an appropriate implementation strategy; select an appropriate expert system tool; and organize the implementation team.

For questions regarding the course content and program structure, please call Jim Davis at (614) 292-0090. To register, call Jody Hadraba at (614) 442-7995 or mail name, title, company, phone number, address, and payment plans for the $695 course fee to Dr. James F. Davis, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, Ohio 43210.

Process Improvement Using Pinch Analysis—The Intensive Four-Day Foundation Course

Linnhoff March, Houston
September 17-20, 1991

The four-day Pinch Analysis (TM) course is for practicing process engineers. It conveys simple and effective principles that are derived from a fundamental logical basis but are aimed at practical application. The material has been proven in many industrial projects across many industries, in the design of new plants and in retrofit work, and in large scale continuous and in batch processes.

You will be presented with a detailed overview of simple and effective principles, including basic concepts (the Pinch concept, energy efficiency targets, the Pinch design method, utility systems); design trade-offs (capital investment targets, capital/energy optimization, plant capacity, process retrofit, debottlenecking); process integration (the process/utility interface, utility system optimization, key process design options, reactors and separators, combined heat and power, and heat pumps); and advanced topics (hydraulic power optimization, design for flexibility, total sites, plant layout, batch process, raw materials efficiency, project execution, and case studies).

To register, please state payment plans for the $1000 course fee and FAX to Alice Spriggs (FAX: 703-777-4145) or mail to Linnhoff March, Inc., 2 Cardinal Park Drive, Suite 205-A, Leesburg, VA 22075.

Advanced Control of Chemical Processes (ADCHEM '91)

Toulouse, France
October 14–16, 1991

This Symposium will address the state of the art of those adaptive, statistical and model based process control methods that are appropriate for process control problems. The Symposium will allow presentation and discussion of papers dealing with new adaptive, statistical, and model based control techniques and applications in chemical and related industries. The International Programme Committee placed the emphasis on practical aspects while selecting the papers. Three survey papers will be presented in plenary sessions. At the symposium, the authors will present summaries of their papers and describe their latest findings. The papers will be open to debate and discussion.

For a complete program listing, registration form, and lit of hotels, please write to ADCHEM '91, L.A.A.S./CNRS, 7 avenue du Colonel Roche, 31077 Toulouse Cedex, France. The registration is FF 2200 before September 16, 1991 and FF 2450 after. Payments will be accepted in French Francs (FF) only. Checks should be made payable to the order of AFCET,

account 502 650 009-02, B.I.M.P., 22 rue Pasquer, F-75008 Paris. It is possible to debit the short course fee to Visa International or Master Card.

Los Angeles AIChE Meeting

November 17–22, 1991

The CAST Division is sponsoring the following sessions at the Los Angeles Annual meeting.

Area 10a: Systems and Process Design

1. Process Synthesis – I
2. Process Synthesis – II
3. Batch Process Design
4. Information Management Systems for Process Design
5. Design and Analysis – I
6. Design and Analysis – II
7. Process Design for Waste Minimization

Area 10b: Systems and Process Control

1. AI Applications in Process Control
2. Recent Advances in Process Control – I
3. Recent Advances in Process Control – II
4. Recent Advances in Process Control – III. [Poster Session]
5. Robust Control
6. Nonlinear Control
7. Control of Discrete Event Processes

Joint Area 10b and Area 10c Sessions:

1. Statistics and Quality Control – I
2. Statistics and Quality Control – II

Area 10c: Computers in Operations and Information Processing

1. Advanced Computer Architectures – I
2. Advanced Computer Architectures – II
3. PC in Chemical Engineering – Visions of the Future
4. Artificial Intelligence in Process Engineering
5. Integrated Approaches to Computer-Aided Process Operations
6. Scheduling and Planning of Process Operations

Area 10d: Applied Mathematics and Numerical Analysis

1. Stochastic Models
2. Complex Chemical Engineering Systems: Chaos, Fractals, and Neural Networks
3. Instabilities and Bifurcations in Chemical Engineering Applications
4. Numerical Methods and Bifurcations in Ordinary Differential Equations
5. PDE Simulations in Chemical Engineering

Optimization of Chemical Processes

Austin, Texas
January 8–10, 1992

Participants who attend this course will be able to formulate optimization problems, analyze typical problems to determine a method of solution, carry out procedures for optimization including linear and nonlinear programming, and apply software programs to obtain solutions to typical industrial problems. The emphasis in this course will be placed on learning optimization procedures which can be used to solve meaningful industrial problems, and to gain experience with optimization software.

For information concerning course content, contact Dr. Thomas Edgar, faculty in-charge, at (512) 471-3080. For registration information, call (512) 471-3506, fax (512) 471-0831, or write to: Continuing Engineering Studies, The University of Texas at Austin, College of Engineering, ECJ 10.324, Austin, Texas 78712.

Singapore International Conference on Intelligent Control and Instrumentation (SICICI '92)

Singapore
February 18-21, 1992

The Conference will be concerned with state-of-the-art in design, implementation and application of Intelligent Control and Instrumentation in continuous process control, manufacturing and related fields. It will provide a forum for presentation and discussion of papers that describe new design approaches, novel applications and experience in implementation of advanced techniques. The program will included invited talks and panel discussions by experts in the field. An industrial exhibition will also be featured in conjunction with the Conference.

The scope of the proposed Conference includes, but is not interested to, the following areas: adaptive control, robust control, robotics, real-time systems, intelligent control, discrete-event control, neural network in control, intelligent process planning, distributed control systems, fault diagnostics and detection, intelligent instrumentation, communications in control, system identification, optimal control, expert systems, CAD, large-scale systems, and motion control.

Early bird registration (before October 31, 1991) is Singapore $600.00. For further information, please contact Secretariat, IEEE Singapore Section, 200 Jalan Sultan, #11-03 Textile Centre, Singapore 0719. Email: FENGHCC@NUS3090.

New Orleans AIChE Meeting

March 29–April 2, 1992

Meeting Program Chairman: Peter R. Pujado, UOP, 25 E. Algonquin Rd., PO Box 5017, Des Plaines, IL 60017-5017, (708) 391-2673, FAX: (708) 391-2253.

The CAST Division is planning the following sessions at the New Orleans National Meeting which were approved at the annual AIChE Programming Meeting in February. Deadlines and final call for papers for this meeting appear later in this issue.

Area 10a: Systems and Process Design

1. **Integration of Process Design, Optimization, and Control.** Henry Chien, Monsanto Company (Chairman).

2. **Training Simulators.** Robert J. Farrell, Polytechnic University, Brooklyn (Chairman) and Sandro Macchietto, Imperial College (Vice Chairman).

3-4 **Process Modeling and Simulation I and II.** Babu Joseph, Washington University (Chairman) and Rodolphe L. Motard, Washington University (Vice Chairman).

Joint Area 10a and Area 10c Session:

1. **Optimization of Batch Unit Operations.** Sandro Macchietto, Imperial College (Chairman) and Lorenz T. Biegler, Carnegie Mellon University (Vice Chairman).

Area 10b: Systems and Process Control

1. **Plant Wide Control.** Irven H. Rinard, City University of New York (Chairman) and James J. Downs, Tennessee Eastman Company (Vice Chairman).

2. **Industrial Applications of Process Control.** David T. Dalle Molle, Amoco Chemical Company (Chairman) and Kenneth A. Bishop, University of Kansas (Vice Chairman).

Area 10c: Computers in Operations and Information Processing

1. **Hazard and Operability Analysis.** Randy A. Freeman, Monsanto Company (Chairman).

2. **Process Data Management and Reconciliation.** Mohinder K. Sood, Mobil Oil Company Ltd. (Chairman) and Granville E. Paules IV, Mobil R&D Corporation (Vice Chairman).

3. **Applications of Neural Networks.** (Rescheduled from Miami Beach Meeting) Venkat Venkatasubramanian, Purdue University (Chairman), and Sanjeev Katti, Dow Chemical Company, (Vice Chairman).

4. **New Environments for Engineering Computations.** Gary D. Cera, Mobil R&D Corporation (Chairman) and Alan B. Coon, Union Carbide Corp. (Vice Chairman).

5. **Software Engineering Tools and Techniques.** Stephen J. Zilora, Creative Software Solutions (Chairman) and Joseph A. Camisa, Exxon Company USA (Vice Chairman).

6. **Technical Desktop Publishing.** Peter R. Rony, Virginia Polytechnic Institute and State University (Chairman) and Richard S. H. Mah, Northwestern University (Vice Chairman).

Area 10d: Applied Mathematics and Numerical Analysis

No Sessions are planned.

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.

If you would like to attend the symposium start planning accordingly. If you are interested in entering a poster or an oral presentation, the Scientific Committee would like to hear from

you as soon as possible. The deadline for the submission of abstracts is May 1, 1991.

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 at vm.uni-c.dk

1992 American Control Conference

Chicago, Illinois
June 24-26, 1992

The following INVITED sessions have been developed for the 1992 ACC:

Modeling and Identification of Chemical Processes. James B. Rawlings (Chairman) and Derrick Kozub (Vice Chairman).

Robust Process Control. Daniel E. Rivera (Chairman) and Jay Lee (Vice Chairman).

Nonlinear Process Control. Francis Doyle (Chairman) and James McLellan (Vice Chairman).

Model Predictive Control (Including Multi-Rate Control). B. Wayne Bequette (Chairman) and Spyros Svoronos (Vice Chairman).

Batch Processes and Discrete Events. Norman Jerome (Chairman) and Jeffrey C. Kantor (Vice Chairman).

Pattern Recognition and Controller Performance Assessment. Mike Piovoso (Chairman) and Tom Marlin (Vice Chairman).

Intelligent Process Control. Karlene Kosanovich (Chairman) and Richard W. Chylla (Vice Chairman).

The session chairs will soon be issuing calls for papers to describe the focus of each of the INVITED sessions listed above. In addition, CONTRIBUTED papers go through a review process, and if accepted for presentation are assigned to a suitable session. There are two types: regular papers (30-minute presentation time) and short papers (15-minute presentation time). If you would like to submit a CONTRIBUTED paper, submit six copies of the manuscript by September 15, 1991 to:

Regular Papers:

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

Short Papers (700 words, 2-3 page summary):

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

Foundations of Computer-Aided Plant Operations (FOCAPO '92)

Summer, 1992

Co-sponsored by CAST Division and CACHE Corporation.

The second Foundations of Computer-Aided Process Operations conference is scheduled for summer 1992. 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 Zurich, 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.

CONTROL SYSTEMS '92

Dream vs Reality: Modern Process Control in the Pulp and Paper Industry

Whistler, BC, Canada
September 28–October 1, 1992

Call For Papers: 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 Cellulosa-ingenjors foreningen, and the Finnish association, Suomen Paperi Insinoorien Yhdistys Ry.

The Conference Chairman is Ron Crotogino 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.

We are currently contacting a number of people from the industry and universities to solicit contributions in order to ensure a successful cross-fertilization of ideas.

Papers or series of papers are sought which trace the development of new control or tuning techniques from their inception to their applications.

Topics to be considered include:

- Selection of control strategies
- Implementation issues of advanced control algorithms
- Applications of adaptive control
- Applications of robust control
- Constrained control
- Monitoring of control loop performance
- Auto-tuning
- Modelling of industrial processes
- Estimation and identification of industrial processes
- Stochastic vs deterministic approach
- Non-linear techniques
- Intelligent control
- SPC/SQC

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. Anyone wishing to present a paper at Control Systems '92 should submit a one-page abstract before November 30, 1991, to:

Alain A. Roche
Program Chairman, CONTROL SYSTEMS '92
Paprican
570 St. John Boulevard
Pointe Claire, Quebec
Canada H9R 3J9

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: _____

I intend to submit a paper for presentation at CONTROL SYSTEMS '92:

_____

Name: _____

Address: _____

Tel. No.: _____

Fax No.: _____

Please also enclose:

1. The names and addresses of any colleagues you think might wish to be informed about this conference.
2. Any suggestions you might have about program content or speakers you might wish to hear.

Miami Beach AIChE Meeting

November 1-6, 1992

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

The CAST Division is planning the following sessions at the Miami Beach Annual Meeting which were approved at the annual AIChE Programming Meeting in February. Deadlines and first 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).

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, Union Carbide Corporation (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).

Joint Area 10a and Area 2 Session:

1. **Design of Separations Systems.** Vasilios I. Manousiouthakis, University of California, Los Angeles (Chairman).

Area 10b: Systems and Process Control

1. **Nonlinear Control.** Vasilios I. Manousiouthakis, University of California, Los Angeles (Chairman) and B. Wayne Bequette, Rensselear 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.** Evanghelos 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. **Nonlinear Time Series.** B. Erik Ydstie, University of Massachusetts (Chairman) and Julio M. Ottino, Northwestern University (Vice Chairman).

2. **Analysis of Complex Systems.** Yannis G. Kevrekidis, Princeton University (Chairman) 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).

Houston AIChE Meeting

March 28–April 1, 1993

Tentative CAST Division programming topics are:

Design for Flexibility

Retrofit Design

New Advances in Process Synthesis

Industrial Applications of CAD – Large Scale Simulators

Simulation of Biological Processes

Design for Safety and Environmental Impact

Design for Lifecycle Operations

Industrial Applications of Process Control

Nonlinear and Predictive Control in Practice

Computer Integrated Manufacturing

Applications of Expert Systems

Experiences with Real Time Packages

Integration of Simulation and Operations

Information Processing through Image Technology

Call For Papers

Final Call for CAST Sessions New Orleans AIChE Meeting March 29–April 2, 1991

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, 1991: 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, 1991: Authors informed of selection and session content finalized.

January 15, 1992: 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, 1992: Submit final manuscript to AIChE.

Area 10a: Systems and Process Design

1. Integration of Process Design, Optimization, and Control.

Chairman

Henry Chien
Monsanto Company
800 N. Lindbergh Blvd.
St. Louis, MO 63167
(314) 694-8274

2. Training Simulators.

Chairman

Robert J. Farrell
Dept of Chemical Eng.
Polytechnic University
Brooklyn, NY 11201
(718) 260-3628
(718) 260-3136 (FAX)

Vice Chairman

Sandro Macchietto
Dept of Chemical Eng
and Chemical Technology
Imperial College
London SW7 2AZ
England
011-44-71-584-1170 (FAX)

3-4. Process Modeling and Simulation I and II.

Papers are sought in all areas of chemical process modeling and simulation. Contributions on applications to industrial processes are particularly welcome. Priority will be given to papers that present novel applications and results.

Chairman

Babu Joseph
Dept of Chemical Eng
Washington University
St. Louis, MO 63130-4899
(314) 889-6076
(314) 726-4434 (FAX)

Vice Chairman

Rodolphe L. Motard
Dept of Chemical Eng
Washington University
St. Louis, MO 63130-4899
(314) 889-6072
(314) 726-4434 (FAX)

Joint Area 10a and Area 10c Session:

1. Optimization of Batch Unit Operations.

Contributions are welcomed from the areas of optimal design of specific batch equipment (e.g. reactors and distillation), planning and scheduling of batch process operations, integration of design and scheduling aspects, synthesis strategies for batch design, dynamic optimization of batch operations, and integration of off-line scheduling and on-line operations.

Chairman

Sandro Macchietto
Dept of Chemical Eng
and Chemical Technology
Imperial College
London SW7 2AZ
England
011-44-71-584-1170 (FAX)

Vice Chairman

Lorenz T. Biegler
Dept of Chemical Eng
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2232
(412) 268-7139 (FAX)
d101lb01@vb.cc.cmu.edu

Area 10b: Systems and Process Control

1. Plant Wide Control.

Of interest are papers emphasizing the development, design, and implementation of plant-wide control strategies. Plant-wide control can be considered as the control of two or more processing units generally with one or more recycle loops. Relevant topics include: identification of measurement and manipulated variable requirements; coordination of local control strategies to achieve overall operational goals for the plant; coordination of inventory control strategy including the location and sizing of tankage; strategies for pairing SISO loops plant-wide; techniques for identifying the need for decentralized MIMO controllers; and strategies for minimizing disturbance propagation through the plant.

Chairman	*Vice Chairman*
Irven H. Rinard	James J. Downs
Dept of Chemical Eng	Tennessee Eastman Co.
City College, City Univ. of NY	P.O. Box 511
New York, NY 10031	Kingsport, TN 37662
(212) 690-4135	(615) 229-5318
(212) 690-4193 (FAX)	(615) 229-6099 (FAX)

2. Industrial Applications of Process Control.

Papers are sought that address the application of novel control strategies in the chemical processing industry. Priority will be given to papers that discuss applications of new control strategies involving adaptive, multivariable, nonlinear, and model-based control. Other topics welcome include intelligent control, supervisory control, and challenging control problems.

Chairman	*Vice Chairman*
David T. Dalle Molle	Kenneth A. Bishop
Amoco Chemical Co.	Dept of Chemical
P.O. Box 3011	and Petroleum Eng
Naperville, IL 60566	University of Kansas
(708) 961-6230	Lawrence, KS 66045-2223
(708) 420-4678 (FAX)	(913) 864-4965
dalle@nap.amoco.com	(913) 864-3199 (FAX)
	kbishop@kuhub.cc.ukans.edu

Area 10c: Computers in Operations and Information Processing

1. Hazard and Operability Analysis.

Chairman

Randy A. Freeman
Monsanto Company – F2WG
800 N. Lindbergh Blvd.
St. Louis, MO 63167
(314) 694-6068

2. Process Data Management and Reconciliation.

Effective modeling, control, and optimization of process plants relies heavily on the quality of measured data and data derived from measurements. Distributed control systems provide enormous quantities of data at a high rate of sampling. Screening of erroneous or inconsistent data is crucial for its use in any of the above applications. This session will focus upon the management and reconciliation of process data through statistical techniques and model-based approaches that integrate the process simulation and/or optimization model with the reconciliation step.

Chairman	*Vice Chairman*
Mohinder K. Sood	Granville E. Paules IV
Mobil Oil Company Ltd.	Mobil R&D Corporation
Coryton Refinery	P.O. Box 1026
The Manorway	Princeton, NJ 08543-1026
Stanford le Hope	(609) 737-4593
Essex SS17 9LL	(609) 737-5047 (FAX)
ENGLAND	
011-44-375-646447	
011-44-375-646741 (FAX)	

3. Applications of Neural Networks.

Chairman	*Vice Chairman*
Venkat Venkatasubramanian	
School of Chemical Eng	Sanjeev Katti
Purdue University	Dow Chemical Company
West Lafayette, IN 47907	Freeport, TX
(317) 494-0734	
(317) 494-0805 (FAX)	
venkat@ecn.purdue.edu	

4. New Environments for Engineering Computations.

Hardware and software advances in the past few years have produced a number of new environments for engineering computations. This session addresses issues arising from the implementation of chemical engineering computations in nontraditional computing environments. Such issues include but are not limited to interoperability, software design and maintenance, portability, computational efficiency, and user interfaces. Applications or descriptions of new environments are sought in programming environments as UNIX, Smalltalk, etc., distributed computing environments including applications using remote servers, applications executing across heterogeneous networks, etc., and user interfaces and visualization tools.

Chairman	*Vice Chairman*
Gary D. Cera	Alan B. Coon
Mobil R&D Corporation	Union Carbide Corp.
P.O. Box 1026	P.O. Box 8361
Princeton, NJ 08543-1026	South Charleston, WV 25303
(609) 737-5299	(304) 747-5470
(609) 737-5325 (FAX)	(304) 747-5448 (FAX)
gdcera@drl.mobil.com	

5. Software Engineering Tools and Techniques.

Software Engineering involves the application of sound engineering principles to the development and management of software applications. This session will present an overview of several of those principles. We are requesting papers which present case studies of software/management efforts with emphasis on some particular aspect of software engineering. The topics may include requirements analysis, prototyping, system design, development environments, quality assurance, delivery, maintenance, version control, metrics, or cost estimation.

Chairman

Stephen J. Zilora
Creative Software Solutions
P.O. Box 192
Flanders, NJ 07836
(201) 927-8233
(201) 927-6741 (FAX)

Vice Chairman

Joseph A. Camisa
Exxon Company USA
P.O. Box 222
Linden, NJ 07036
(201) 474-7340
(201) 474-7713 (FAX)

6. Technical Desktop Publishing.

Papers are solicited that provide practical information concerning near term issues associated with the use of "technical desktop publishing" – namely, the desktop publishing of technical documents that include equations, graphs, tables, and text - in industry, government, and academia. The session seeks to address the following issues: hardware and software availability; manuscript layout and graphical design considerations; document structure and retrieval; and distribution and marketing. Of special interest are publishing issues, on-line textbooks, experiences with electronic technical publishing, industrial in- house publication, editing, document structure, information capture, etc.

Chairman

Peter R. Rony
Dept of Chemical Eng
Virginia Polytechnic Inst.
and State University
Blacksburg, VA 24061-6496
(703) 231-7658
(703) 231-7826 (FAX)
rony@vtvm1.cc.vt.edu

Vice Chairman

Richard S. H. Mah
Dept of Chemical Eng
Northwestern University
Evanston, IL 60208-3120
(708) 491-5357
(708) 491-3728 (FAX)
dick_mah@nuacc.bitnet

Final Call for Papers
1992American Control Conference
Chicago, Illinois
June 24-26, 1992

Invited Session Sponsored by AIChE

The names, addresses, and telephone numbers of the session chairmen are given below, as are brief statements of the session topics. Prospective session participants are encouraged to observe the following deadlines.

The following deadlines apply:

August 15, 1991: To have a paper considered for the session, please submit a 500 word abstract (electronically or by mail) to both session chairmen. This is a "real" deadline.

January 21, 1992: Authors notified and authors' kits distributed.

March 1, 1992: Deadline for typed mats for Proceedings.

Robust Process Control

Papers are sought that address both theoretical and practical developments in the field of robust process control. Topics of interest include but are not limited to: design and analysis of robust control systems, robustness of decentralized, constrained, and inferential control systems, computation of error bounds, relationships to system identification, and applications of robust control theory to industrial processes. Papers that focus on how to make robust control design a more commonplace practice by process control engineers are especially welcome.

Chairman

Daniel E. Rivera
Dept of Chemical, Bio
and Materials Engineering
Arizona State University
Tempe, Arizona 85287-6006
(602) 965-9476
(602) 965-2910 (FAX)
rivera@asuvax.egs.asu
.edu (e-mail)
rivera@envs07.cim.eas.asu
.edu (alternative e-mail)

Co-Chairman

Jay Lee
Dept of Chemical Eng
Auburn University
Auburn, AL 36489-5127
(205) 844-2060
(205) 844-2063 (FAX)
jhl@eng.auburn.edu

Batch Processes and Discrete Events

Papers are sought that address research problems in the control and operation of batch processing and discrete event dynamical systems. We wish to provide a forum for

describing industrial problems, case studies, and the description and application of new theoretical results. Topics include but are not limited to the synthesis and analysis of logic based control systems, control verification, and performance analysis. Theoretical tools would include queuing theory, Petri nets, and logic based algorithms.

Chairman

Norman F. Jerome
Amoco Research Center
Mail Code B-3
PO Box 3011
Naperville, IL 60566-7011
(708) 420 3776
(708) 961 6250 (FAX)
njerome@nap.amoco.com

Co-Chairman

Jeffrey C. Kantor
Dept of Chemical Eng
Univ. of Notre Dame

Session on Intelligent Process Control

Papers are requested that address both theoretical and practical developments in the area of intelligent process control. Topics of particular interest include but are not limited to: heuristic-based algorithms, neural networks, statistical techniques, smart instruments, and logic-based control systems. Applications of intelligent control to industrial processes are especially welcome.

Co-Chairman

Karlene A. Kosanovich
E. I. Du Pont de Nemours
Exp. Stn Bldg 001/212
P.O. Box 80101
Wilmington, DE 19880-0101
(302) 695-4318
(302) 695-2645 (FAX)
kosanoka@esvax.dnet
.dupont.com

Co-Chairman

Richard W. Chylla
S.C. Johnson Wax
1525 Howe St.
Racine, WI 53403
(414) 631-3568
(414) 631-3181 (FAX)

Nonlinear Process Control

Papers are sought that address new theoretical results in nonlinear process control and applications of nonlinear control to chemical engineering systems. Priority will be given to papers which address differential geometric methods, generic model control, nonlinear formulations of model predictive control, adaptive nonlinear control, sliding mode control, and robustness issues. In particular, papers are sought which discuss in detail industrial applications of these techniques.

Co-Chairman

Francis J. Doyle III
210-41 Caltech
Pasadena, CA 91125
(818) 356-4869
(818) 568-8743 (FAX)
fjd@imc.caltech.edu

Co-Chairman

P. James McLellan
Dept. of Chem. Eng.
Queen's University
Kingston, Ontario
Canada K7L 3N6
(613) 545-6343
(613) 545-6637 (FAX)
mclellan@pcontrol.chee
queensu.ca

Model Predictive Control

Papers which demonstrate advances in model predictive control theory or applications are invited. We are particularly interested in multi-rate and nonsquare systems.

Co-Chairman

B. Wayne Bequette
Dept of Chemical Eng
Rensselaer Polytechnic Inst
Troy, NY 12180-3590
(518) 276-6683
(518) 276-4030 (FAX)
bequette@bequette.che
.rpi.edu

Co-Chairman

Spyros A. Svoronos
Dept of Chemical Eng
University of Florida
Gainesville, FL 32611
(904) 392-9101
(904) 392-9513 (FAX)
o9999tv@ufpine.bitnet

Modelling and Identification of Chemical Processes

This session is being organized to overview modelling and identification approaches that are used in controller design and monitoring. Relevant issues include the level of modelling detail that is required for effective control, whether linear or nonlinear models should be employed, efficient methods for identifying models with a limited amount of process data, the sensitivity of the control performance to the degree of approximation in the model, and methods for identifying and exploiting the uncertainty in the model. Papers dealing with the issues of model reduction, model-based data reconciliation, and novel uses of statistics in analyzing process data are also welcome.

Co-Chairman

Prof. James B. Rawlings
Dept of Chemical Eng
The Univ. of Texas at Austin
Austin, Texas 78712
(512) 471-4417
(512) 471-7060 (FAX)
jbraw@che.utexas.edu

Co-Chairman

Dr. Derrick Kozub
Shell Development Co.
Westhollow Research Ctr
P.O. Box 1380
Houston, Texas 77001
(713) 493-8028
(713) 493-8508 (FAX)

First 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.

Chairman

Babu Joseph
Department of Chemical Engineering
Washington University
St. Louis, MO 63130-4899
(314) 889-6076
(314) 726-4434 (FAX)

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.

Chairman

Joseph F. Pekny
School of Chemical Eng
Purdue University
West Lafayette, IN 47907
(317) 494-7901
(317) 494-0805 (FAX)
pekny@ecn.purdue.edu

Vice Chairman

Amy R. Ciric
Dept of Chemical Eng
University of Cincinnati
Cincinnati, OH 45221-0171
(513) 556-2763
(513) 556-3473 (FAX)

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 account for uncertainties in various parts of the overall model such as equipment, planning schedule, utilities, and product market are also of interest.

Chairman

Heinz A. Preisig
School of Chemical Eng
and Industrial Chemistry
Univ. of New South Wales
P. O. Box 1
Kensington, N.S.W. 2033
AUSTRALIA
61-2-697-2222 x4307
61-2-662-1587 (FAX)
90b0006@csdvx2.accu.csd
.unsw.oz.au

Vice Chairman

Michael F. Malone
Dept of Chemical Eng
University of Massachusetts
Amherst, MA 01003-0011
(413) 545-0838
(413) 545-1647 (FAX)
mmalone@ecs.umass.edu

4. Process Synthesis

Chairman

Rakesh Govind
Dept of Chemical Eng
University of Cincinnati
Cincinnati, OH 45221-0171
(513) 566-2666
(513) 556-3473 (FAX)

Vice Chairman

D. Lionel O'Young
Union Carbide Corporation
P.O. Box 8361
South Charleston, WV 25303
(304) 747-5020

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.

Chairman

Christodoulos A. Floudas
Dept of Chemical Eng
Princeton University
Princeton, NJ 08544-5263
(609) 258-4595
(609) 258-0211 (FAX)

Vice Chairman

William L. Luyben
Dept of Chemical Eng
Lehigh University
Bethlehem, PA 18015-4791
(215) 758-4256
(215) 758-5057 (FAX)

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

Lyle H. Ungar
Dept of Chemical Eng
University of Pennsylvania
Philadelphia, PA 19104-6393
(215) 898-7449
(215) 573-2093 (FAX)
ungar@cis.upenn.edu

Vice Chairman

James F. Davis
Dept of Chemical Eng
Ohio State University
Columbus, OH 43210-1180
(614) 292-0090
(614) 292-9021 (FAX)
davis_j@kcgl1.eng.ohio-state.edu

Joint Area 10a and Area 2 Session:

1. Design of Separations Systems

Chairman

Vasilios I. Manousiouthakis
Dept of Chemical Eng
University of California
Los Angeles, CA 90024-1592
(213) 825-9385
(213) 206-4107 (FAX)

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.

Chairman

Vasilios I. Manousiouthakis
Dept of Chemical Eng
University of California
Los Angeles, CA 90024-1592
(213) 825-9385
(213) 206-4107 (FAX)

Vice Chairman

B. Wayne Bequette
Dept of Chemical and Environmental Eng
Rensselear Polytechnic Inst
Troy, NY 12180-3590
(518) 276-6683
(518) 276-4030 (FAX)
bequette@bequette.che.rpi.edu

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.

Chairman

James B. Rawlings
Dept of Chemical Eng
University of Texas
Austin, TX 78712-1062
(512) 471-4417
(512) 471-7060 (FAX)
jbraw@che.utexas.edu

Vice Chairman

Michael Nikolaou
Dept of Chemical Eng
Texas A&M University
College Station, TX 77843-3122
(409) 845-0406
(409) 845-6446 (FAX)
m0n2431@tamusigma.bitnet

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.

Chairman

Evanghelos Zafiriou
Systems Research Center
University of Maryland
College Park, MD 20742
(301) 405-6625
(301) 405-6707 (FAX)
zafiriou@cacse.src.umd.edu

Vice Chairman

Richard W. Chylla
S. C. Johnson & Son, Inc.
1525 Howe Street, M.S. 305
Racine, WI 53403-5011
(414) 631-3568

Chairman

Ignacio E. Grossmann
Dept of Chemical Eng
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2228
(412) 268-7139 (FAX)
d391gr99@vb.cc.cmu.edu

Vice Chairman

Angelo Lucia
Dept of Chemical Eng
Clarkson University
Potsdam, NY 13699-5705
(315) 268-6674
(315) 268-3841 (FAX)

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.

Chairman

Stephen E. Zitney
Cray Research Inc.
655E Lone Oak Drive
Eagan, MN 55121
(612) 683-3690
(612) 683-3099 (FAX)
sez@cray.com

Vice Chairman

Anthony Skjellum
Computing & Mathematics
Research Division
Lawrence Livermore
National Laboratory
P.O. Box 808
Livermore, CA 94551
(415) 422-1161
(415) 423-2993 (FAX)
tony@lll-crg.llnl.gov

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.

Cochairman

Iori Hashimoto
Chemical Eng Dept
Kyoto University
Yoshida-Honmachi Sakyo-ku
Kyoto, 606 JAPAN
075-753-5560
075-761-7695 (FAX)

Cochairman

G. V. Reklaitis
School of Chemical Eng
Purdue University
West Lafayette, IN 47907
(317) 494-4075
(317) 494-0805 (FAX)
reklaiti@ecn.purdue.edu

Area 10d: Applied Mathematics and Numerical Analysis

1. Nonlinear Time Series.

Chairman

B. Erik Ydstie
Dept of Chemical Eng
University of Massachusetts
Amherst, MA 01003-0011
(413) 545-2388
(413) 545-1647 (FAX)
ydstie@ecs.umass.edu

Vice Chairman

Julio M. Ottino
Dept of Chemical Eng
Northwestern University
Evanston, IL 60208
(708) 491-7398
(708) 491-3728 (FAX)

2. Analysis of Complex Systems.

Chairman

Yannis G. Kevrekidis
Dept of Chemical Eng
Princeton University
Princeton, NJ 08544
(609) 258-2818
(609) 258-6744 (FAX)
yannis@marilyn.princeton.edu

Vice Chairman

Hseuh-Chia Chang
Dept of Chemical Eng
University of Notre Dame
Notre Dame, IN 46556
(219) 239-5697
(219) 239-8366 (FAX)

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.

Chairman

Joseph F. Pekny
School of Chemical Eng
Purdue University
West Lafayette, IN 47907
(317) 494-7901
(317) 494-0805 (FAX)
pekny@ecn.purdue.edu

Vice Chairman

Ross E. Swaney
Dept of Chemical Eng
University of Wisconsin
Madison, WI 53706
(608) 262-3641
(608) 262-5434 (FAX)
swaney@chewi.che.wisc.edu

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.

Chairman

Jeffrey C. Kantor
Dept of Chemical Eng
University of Notre Dame
Notre Dame, IN 46556
(219) 239-5797
(219) 239-8366 (FAX)
jeff@darwin.cc.nd.edu

Vice Chairman

Michael F. Doherty
Dept of Chemical Eng
University of Massachusetts
Amherst, MA 01003-0011
(413) 545-2359
(413) 545-1647 (FAX)
doherty@ecs.umass.edu

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.

Chairman

George D. Byrne
Exxon Research and
Engineering Company
Route 22E
Annandale, NJ 08801
(201) 730-3115
gdbyrne@erenj.bitnet

Vice Chairman

Bruce A. Finlayson
Dept of Chemical Eng
University of Washington
Seattle, WA 98195
(206) 543-2250
(206) 543-3778 (FAX)
finlayson@chevax.cheme
.washington.edu

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

1992 AWARD NOMINATION FORM*

A. BACKGROUND DATA

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

2. Name of Nominee _____ Date of Birth _____

3. Present Position (exact title)

_____

4. Education:

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

5. Positions Held:

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

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

7. Technical and Professional Society Memberships and Offices

8. Sponsor's Name and Address

_____

_____

_____

_____ Sponsor's Signature

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

B. CITATION

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

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

C. QUALIFICATIONS

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

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

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

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

4. Other pertinent information.

D. SUPPORTING LETTERS AND DOCUMENTS

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

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

For the next five months, please send the completed 1992 award nomination form and supplemental sheets to the CAST Division 2nd Vice Chairman, Professor Michel F. Doherty, Chemical Engineering Department, University of Massachusetts, Amherst, MA 01003. Phone: (413) 545-2359, FAX : (413) 545-1647.

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