Computing and Systems Technology Division Communications

Volume 12, Number 1, March 1989

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programming information obtained during the previous March AIChE meeting.

October 1: Request updated information from Area Chairmen for Fall CAST Executive Committee Meeting Programming Board Report and MPC discussions. Send reminder to Area Chairmen for CAST Communications Winter Issue (tentative Fall Program 2 years out and Spring Program First Call 1.5 years out). Remind Area Chairmen who do not hold spring planning meetings to plan 2.5 years out. Send Area Chairmen updated CAST programming history.

November 1: Prepare Fall CAST Programming Board Report. Prepare Fall CAST Editorial Board Report.

November: Attend AIChE Annual Meeting, CAST Executive Committee Meeting, Area Programming Planning Meetings, Future Meetings Roundtable (MPC discussions), and National Program Committee Meeting. Hold Programming Board Meeting. Confirm MPC schedules and deadlines.

December 1: Deadline to receive material from Area Chairmen for CAST Communication Winter Issue. Receive minutes from Area Programming Planning Meetings, including tentative session titles and chairmen.

December 15: Send updated program information to Meeting Program Chairmen, if not submitted at roundtable.

December: Prepare edited programming material for CAST Communications Winter Issue.

In making this change, the Publications and Programming board chairmen suggest the following advantages:

- Both industrial and academic CAST Division members will be given information on forthcoming AIChE meeting sessions with sufficient advance notice to give them the maximum opportunity to participate.

- The new publication schedule takes better advantage of the streamlined set of deadlines for presentations at AIChE meetings. For example, for the San Francisco meeting, all members of the Division are reading the Calls in early February, and have until the middle of April to submit abstracts to session chairman.

- The Newsletter would be able to present the latest information concerning future meeting CAST session scheduling. Area programming committee meetings are held at the national meetings. Publication of the newsletter after each national meeting will permit inclusion of committee decisions and plans.

- The editor would have an opportunity to convey timely information that he or she gathers at each national meeting, a time when a significant portion of CAST Division business is conducted.

- The CAST Division chairman would have an opportunity to convey his or her thoughts at the conclusion of each semi-annual CAST Executive Committee meeting.

To repeat comments made in the "About This Issue" editorial: This issue will be one of two to be published this year: Volume 12, No. 1, the Fall 1988 issue, delayed significantly to accommodate the Calls for Papers for the 1989 San Francisco AIChE meeting and combined with what would have been the Winter 1989 issue; ; and Volume 12, No. 2, also known as the "Summer 1989" issue, which will be published on time in August 1989 and will contain the Award Address (including copies of his illustrations) by Professor J. D. Seader, "Computers in Chemical Engineering Education," at the CAST Division banquet at the Washington D.C. AIChE meeting. This revised schedule has been developed with the cooperation of both the Publications and the Programming Board chairmen. By the end of the summer, we hope to have all of the CAST programming area chairmen linked electronically by BITNET. A listing of tentative programs, first calls, final calls, and a program schedule for the next meeting will be updated every several months and made available to all CAST Division members (who have access to BITNET) on the LSUCHE GRAND file server at the Department of Chemical Engineering, Louisiana State University. We are still hoping that AIChE headquarters in New York will be able to gain access to a local BITNET node.

We believe that we have an interesting issue for you. In addition to Calls for Papers; announcements of meetings, conferences, short courses, and workshops; and announcements of the 1988 CAST Division award winners; we have two feature articles, a contribution from one of the sponsors of our Division awards, two advertisements, thanks from the Washington D.C. Meeting Program Chairman, and a message from the Chairman of the AIChE Management Division.

First, we would like to thank Kay Kuenker and Gary Blau for writing an original article on Dow's exciting new software, SimuSolv. Second, we would like to thank Robert Simon at the National Research Council for allowing us to have permission to publish Chapter 8 from **Frontiers in Chemical Engineering: Research Needs and Opportunities** (Copyright 1988 by the National Academy of Sciences). Though most academic members of the CAST division have seen the full report, it is our opinion

that not all industrial members have done so. We shall publish this chapter in its entirety in this issue. If you would like a copy of the full report, send $19.95 for FRONTP (paperbound) or $29.95 for FRONTC (hardbound) to National Academy Press, 2101 Constitution Avenue, NW, Washington, DC 20418. Prices apply only in the United States, Canada, and Mexico, and are subject to change without notice. You can also send a letter, along with your VISA/Master Card/American Express account number, requesting the publication.

Third, we are publishing, for the first time, advertisements – from Dow Chemical Corporation and Batch Process Technologies, Inc. – as a service to CAST Division members. The ability to run ads finally was approved by AIChE Council last spring. Advertisement policy for CAST Communications, as communicated by Diane Foster on February 7, 1989, will be as follows: (1) CAST Communications will not solicit advertisements from current or recent advertisers in the AIChE flagship magazine, CEP. If such groups wish to advertise in this newsletter, CEP must approve the request in advance. They will be offered a special discount of 10% of the total advertising cost in CEP and CAST Communications combined. The objective is for advertisements in CAST Communications to augment rather than interfere with advertising in CEP. (2) The Treasurer of the CAST Division will bill and collect advertising revenue associated with ads in CAST Communications. (3) The CAST Division will be required to keep proper records of advertising revenue and expenses. A form will be provided to the Division by AIChE headquarters. (4) The cost of advertising, in the absence of discounts, in CAST Communications will be:

$600	One full page, black and white
$350	One half page, black and white
$250	One-third page, black and white
$450	Two-thirds page, black and white
$400	One half page island, black and white
extra $250	Page or fraction thereof, standard 2nd color
extra $300	Page or fraction thereof, matching 2nd color that requires a special ink
extra $700	Page or fraction thereof, 4-color ad on glossy paper

The fact that in this issue there is both a feature article and an advertisement from Dow Chemical Corporation is coincidental. The editors have Gary Blau to thank for providing us with the incentive, more than one year ago (before the invitation was extended to him to contribute an article on SimuSolv), to request AIChE Council to consider newsletter advertising policy. Advertisements will be decoupled from editorial content, which will be judged separately on merit. In other words, if you are in industry and wish to contribute an article on a new item of computer hardware, software, or systems, you are not required to purchase an ad in order to do so.

We would like to thank two outgoing CAST officers, Mac Clarke, CAST Division chairman, and Rex Reklaitis, Programming Board chairman, for their contributions to and support of the newsletter. We welcome our new officers; their photographs and biographical sketches are provided elsewhere in this issue. We also welcome our new Council Liaison, Tom Edgar.

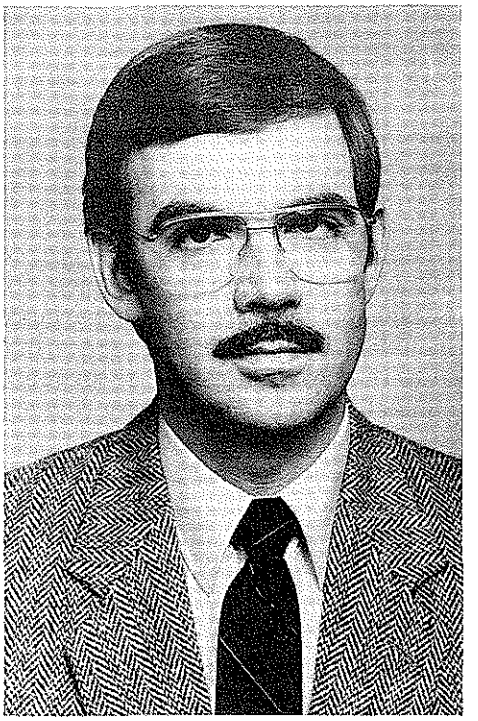
New CAST Division Officers Elected,

by W. MacMaster Clarke

The CAST Division officers election, as certified by Gordie Ellis of the AIChE New York office, are as follows: 593 valid ballots returned of 1848 sent. Elected were:

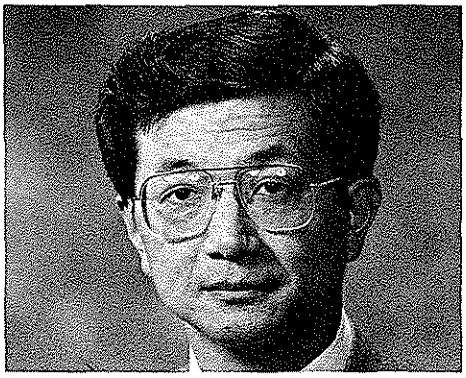
G. V. (Rex) Reklaitis, Second Vice Chairman

Rex (PhD, Stanford University) is currently Professor and Head of the School of Chemical Engineering at Purdue University. He recently completed a term as Assistant Dean of Engineering, Graduate Education and Research. Prior to that, Rex was a Senior Fullbright Lecturer at Vilnius State University and Lithuanian Academy of Science. His research interests include process design and simulation, particularly of batch and semi-continuous processes, for which in 1984 he received the CAST Computing in Chemical Engineering Award. Rex is the co-editor of *Computers and Chemical Engineering*, and was the co-chairman of the first FOCAPO conference. He is a Trustee and has served as President of the CACHE Corporation. He was a CAST Division Director from 1981-83, CAST Area 10c Programming Chairman from 1982-84, and is the retiring CAST Division Programming Board Chairman.



Henry H. Chien, Director (1989-1991)

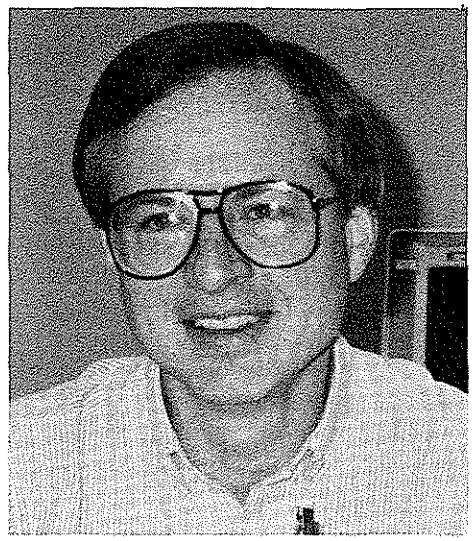
Henry (PhD, University of Minnesota) is currently a Senior Fellow, Engineering Technology Department, Monsanto Chemical Company. He has been actively involved in the development of computer-aided process engineering tools for design, simulation, and optimization as well as process dynamics and control. He recently served on the ASPEN Project industrial board, and also on a subpanel of the Amundsen Committee. Henry has organized several sessions at AIChE meetings, and was co-chairman of the FOCAPD-83 conference. He has served on the CAST Area 10A Programming Committee since 1978.



A. L. (Pete) Parker (1989-1991)

Pete (PhD, University of Wisconsin) is currently Manager of Planning and Economics at the Norco Manufacturing Complex of Shell Oil Company. His previous experience included work in process engineering, and the development of process simulators. His interests are refinery planning and scheduling tools, and plant-wide information systems. Pete has been an active member of CAST since its inception, chairing symposia on workstations, retrofitting, and computer-aided engineering. He currently serves on the CAST Area 10c Programming Committee.

Rex has resigned as the CAST Programming Board Chairman. His



replacement is the past CAST chairman for 1988, Jeffrey J. Siirola.

Other changes in the CAST Division Executive Committee are listed on the inside front cover.

Editorial

by Peter R. Rony

It will now be possible to advertise within the pages of CAST Communications, a decision approved by Council last spring. The rates will be set by AIChE headquarters; the cost per page is as listed on page 2 of this Newsletter. One of the general guidelines that apply to such advertising is that it does not diminish the advertising potential in CEP. Bundled advertising rates, in which an advertiser appears both in CEP and CAST Communications, will be possible. Please contact AIChE headquarters in New York if you are interested. Whatever funds the Division receives from advertising revenue will be used to reduce the cost of the newsletter, which is now the single largest expense of the Division.

During the Washington DC AIChE meeting, I had the opportunity to attend the programming committee meetings of areas 10a, 10b, and 10c. I was impressed by the large number of committee participants–twenty or more–at each meeting and their effectiveness at developing program ideas and recommended session chairmen for CAST Division sessions at the 1990 Orlando and Chicago meetings. The CAST Division probably programs further in advance than any other Division in the Institute. All programming areas solicit your suggestions concerning sessions that you would like to see at future meetings, and solicit your participation as speakers in planned sessions.

Congratulations are extended to a former Chairman of the CAST Division, Tom Edgar, on his election as Director of the Institute. Tom becomes our new representative on Council. Stan Proctor, our representative for the last several years, stopped by at the CAST Executive Committee in Washington DC and gave us the benefit of his perspective of Council decisions. Stan has done this at every national meeting, despite a very busy schedule.

The results of the CAST Membership Survey are being published in this issue. 63 members out of 200 contacted replied. The Division currently has approximately 1800 members

This issue contains a new "first," thanks to Mark Kramer (MIT) and Gary Cera (Mobil), both of whom have provided their FAX numbers. We encourage other contributors to this newsletter to do so in the future. Facsimile transmission is becoming more popular as a standard and widespread method of communicating written information. For the transmission of paper text and images, it is a non-intrusive alternative to slow postal delivery, express mail, or electronic communications. My FAX number is (703) 961-7826.

More faculty in academia are acquiring BITNET userids for use with

this international wide area network. I have recently updated a nicknames listing for IBM mainframes, and have counted more than 400 BITNET userids. Although BITNET is reserved primarily for organizations that have a strong academic or educational component (some industrial organizations qualify), it is possible to access BITNET through network gateways tied to networks such as INTERNET, CSNET, ARPANET, and so forth. CAST Communications has been available in electronic form since last spring at the GRAND at LSUCHE node at Louisiana State University. Some of the GRAND files are maintained locally in Blacksburg and are available by sending a message to RONY at VTVM1. For example, the IBM nicknames list eliminates the need to have written listings of sometimes complex and difficult-to-remember BITNET userids. CAST Division members who are active in programming activities perhaps could acquire a BITNET userid through a colleague at a local university. Tom Edgar will determine whether any of the engineering societies located in the New York Engineering building have a BITNET node. If so, perhaps AIChE could tie into the network at very little cost and effort.

Ralph Mordo, Manager of Information Services at AIChE headquarters in New York, has an MCI account. Because of a decline in Institute income, there will be no special AIChE initiatives in the area of electronic mail and bulletin boards during the forthcoming year. AIChE funds are being reallocated to provide support for meeting programming in the Institute, for example, for the coordination of programming activities. The Institute lost money on the preprinting of papers at the New York AIChE meeting last year. The full address of authors may in the future be published either in the meeting program booklet or in the abstracts summary. There will be a demonstration of the GRAND wide-area network at the San Francisco AIChE meeting.

Henry McGee, Meeting Programming Chairman for the Washington DC meeting, extends his thanks to CAST Division members who participated in all aspects of the CAST sessions, which were well attended. CAST ranks high on his list as one of the most effective divisions in the Institute.

At the CAST Division Dinner in Washington DC, Professor J. D. Seader gave an entertaining lecture as the CAST Computing in Chemical Engineering award recipient. After listening to his presentation at one of the CAST Area 10d sessions, it is clear that Bob is the "chemical engineer most likely to make it to infinity (positive or negative) and back and live to tell the tale." Ask him to discuss his "boomerang" technique. His Award Address will be published in the forthcoming Summer 1989 issue of CAST Communications.

At my table during the CAST Division Dinner, we got to talking about the various written and verbal subterfuges that we employed fifteen to twenty-five years ago in order to acquire a minicomputer for our research / development efforts. Michael A. Burroughs remembered when he called a computer a "monitor stand." Recent chemical engineering graduates may not realize that at one time it was highly unusual, even suspect, for an individual or small group to have his or its "own" computer. As a low-key contest–the first in the history of this newsletter–I would like to ask Division members to probe their colleagues for anecdotes associated with the ordering of "personal" or "group" minicomputers during a period when it was difficult to do so. I would like to identify the most unusual description, or name, of a successfully ordered computer in industry during the period, 1962 to 1974. A panel of the CAST editorial board, and CAST Executive committee, will select the winners; our decision will be final. The deadline for entries is April 31, 1989. Perhaps, as first prize, we could offer a one-year subscription to CAST Communications. Second prize could be a two-year subscription to this Newsletter! A minimum of twenty entries will be needed in order to have a viable contest, so please submit, or have a colleague submit, an entry even if you or he are not convinced that the description is a likely winner. Membership in the AIChE or the CAST Division is not a requirement for participation. Send anecdotes to me in Blacksburg.

One of the papers at the Washington DC meeting that I liked the most was the Area 10d paper, "The Use of Hamiltonian Mechanics and Symmetries in the Analysis of Chaotic Mixing and Two-Dimensional Flows," by P. D. Swanson and J. M. Ottino (University of Massachusetts). I was subsequently informed that work conducted in Dr. Ottino's laboratory will be the cover story in the January 1989 issue of Scientific American. It is uncommon for chemical engineers to be able to communicate to the public through this magazine, so kudos and hurrahs are conveyed to Professor Ottino and his colleagues. The article is entitled, "The Mixing of Fluids," and can be found on page 56.

The 1990 Chicago AIChE meeting may prove to be a special occasion for the CAST Division. The proximity of Fermilab, a national supercomputer center, and other centers of computer activity provide an opportunity to make "computing" one of the themes of this meeting.

For a future issue of CAST Communications, we would like to have a feature article on the subject of "graphics supercomputing and scientific visualization." This, by the way, was the subject of a series of Stellar seminars given during October 1988 in New York City, Reston, Ithaca, Surrey, and Munich by Stellar Computer Inc., 85 Wells Avenue, Newton, MA 02159, (617) 964-1000. In

the future, it is likely that chemical engineering simulations of great complexity will become more visually oriented.

See you in Houston.

CAST Membership Survey, Summer 1988

by Bruce Finlayson

Tabulation by per cent of respondees (% of 63). Total responses = 63 out of 200 surveys. Membership, approximately 1800.

CAST needs your help. We are surveying a small, randomly selected group of CAST members. If you take a few minutes now and answer the questions below it will improve CAST by letting us focus on projects that are significant to the membership. Since the sample size is small, your reply is important. Please help.

Profile

1. How long have you been a CAST member?

   [27%] Less than 2 years
   [46%] 2-5 years
   [21%] 5-10 years
   [5%] Longer

2. Do you work in:

   [27%] Academia
   [76%] Industry
   [2%] Government
   [0%] other?

AIChE Meetings

3. How long since you have been to a National or Annual AIChE meeting?

   [27%] Never
   [33%] One year
   [13%] Two years
   [10%] Three to five years
   [17%] Longer than five years ago

4. The last six AIChE meetings were at the following locations. Circle the ones you attended.

   [24%] New Orleans
   [16%] New York
   [8%] Minneapolis
   [14%] Houston
   [14%] Miami Beach
   [6%] Boston

5. How do you use the information presented in CAST sessions at the AIChE meetings? (Mark all that apply)

   [13%] Don't use it
   [59%] For general information – to see what the field is doing
   [48%] Stimulates my thought for new projects/directions
   [22%] Apply results to my daily work

6. When a paper is presented at a meeting how important is it that printed copies of the papers be available?

   [60%] Very
   [27%] Somewhat
   [2%] Not at all

7. Have you ever attended a FOCAP meeting?

   [11%] Yes
   [81%] No

Newsletter

8. Do you read the CAST Newsletter?

   [2%] Never
   [29%] Peruse it
   [65%] Read articles/meeting announcements

9. What features do you find most interesting/helpful to you?

Features of newsletter found interesting/helpful:

- Good and short; source of a lot of information
- Announcements/summaries of papers
- Announcements
- In-depth articles on new areas, e.g. parallel computing
- Future meetings
- Software reviews; feature articles
- Meeting announcements (2)
- Article; reviews and forum
- Varies from issue to issue
- Process control/optimization
- Articles
- Technical papers
- All
- Meeting announcements and abstracts
- Industrial applications
- Technical articles and announcements
- Review of articles and meeting notices
- Short pages, reports of meetings
- Nothing stands out
- General technical/computing
- Articles, reports
- Computing/simulation
- Articles
- Computational fluid mechanics/heat transfer
- Research/applications/people
- Seminars, meeting announcements
- Real world problems and solutions
- Announcements and directions
- Application notes, discussions, workstation concepts, etc.
- Control related
- Have never received it (3)
- Applications
- General interest

Awards

10. Have you ever participated in the awards process?

    [6%] Nominated someone

[10%] Wrote supporting letters
[5%] Served on review committee

11. Do you know how to nominate someone?

[16%] Yes
[84%] No

Electronic mail/bulletin board

12. Would you like to use electronic mail/bulletin boards to find out about AIChE meetings? Mark all that apply.

[51%] To see what sessions are planned for next year
[48%] To see the titles of papers presented at the next meeting
[49%] To see the extended abstracts of papers at the next meeting

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On-Line and On-Time: MCI Mail and BITNET for Industrial Members of the CAST Division

by Peter R. Rony

The following communication recently appeared in the press under the heading, *On Line and On Time*. The clipping was sent to me by Tom Edgar.

"AIChE now subscribes to MCI Mail, the electronic mail service which can send messages quickly and efficiently via computer. This service can transmit memos, questions, or even copy for AIChE publications (such as AICHExtra) electronically or on paper.

"To utilize MCI Mail, all you need is a personal computer and a modem. Dial your electronic mail phone number and address your mail to us using our MCIID number, 346-6087. The message will enter an electronic "in-box" at AIChE. From that central computer, your message will be delivered to whomever you want at National Headquarters. If you need to send to more than one person, you can copy in the extra recipients without retyping the message.

Subscribers to other electronic mail services, such as AT&T or CompuServe, may also be able to utilize AIChE's MCI line. Check with your local electronic mail representative for information on how to access our system.

"In addition to MCI Mail, AIChE also has a FAX machine. Material can be FAXed to us by dialing (212) 752-3294."

I have an MCI account; the "customer name" is Peter R. Rony and the ID is 351-4388. I credit Patrick H. McNamara, an AIChE member, for providing the incentive for me to join MCI Mail. My strong suspicion is that the new AIChE MCI Mail account service described above also is a result of Pat's efforts, who suggested it in an April 19, 1988 letter to James Mathis. Pat is very knowledgeable about this service. You can reach him at The McNamara Grassroots Group, Inc., 450 5th Street, N.W., Washington, DC 2001, (202) 546-3509. Pat's MCI ID is 219-4743.

I encourage industrial members of the CAST Division to send me messages over MCI Mail or BITNET. During the past six months, I have not read many messages nor used MCI Mail very much, but could do so should the need arise. To use MCI Mail, you must have the proper hardware and communications protocol:

Modem 212A compatible
110, 300, or 1200 baud
Full duplex
8 data bits
No parity
Xon and Xoff protocol
End line with a carriage return

To access MCI Mail: Dial MCI Mail's local access number. Connect the phone to your modem and press RETURN. (For 300 baud, RETURN, pause, RETURN) Enter your user name and password when asked Press RETURN after you type each one. For assistance, call Customer Support toll-free at 800-444-6245. In Washington, DC, call 833-8484. The MCI address is 1900 M Street, NW, Box 1001, Washington DC 20036.

I recently received information from MCI concerning (1) Preferred pricing for FAX transmission–40 messages per month for $10; (2) free Advanced service to be installed by February 6, 1989–provides the commands FORWARD, INCLUDE, and DOC and the ability to store up to 15 letterheads and signatures; and (3) Free 800 access–it is now free to connect to MCI Mail from anywhere in the United States over 800-234-6245 for 300 and 1200 baud, 800-456-6245 for 2400 baud, and 800-825-151 for users of Lotus Express and Desktop Express (300, 1200, 2400 baud).

You will need software to organize your communication needs and activities. One possibility is Lotus Express for MCI Mail. I have a brochure on this product, but no knowledge of its price, which is probably several hundred dollars. Contact Lotus Development Corporation, 55 Cambridge Parkway, Cambridge, MA 02142. Another possibility is the shareware program, QMODEM. This software is available on computer bulletin boards. If you download it, test it, like it, and use it, you are requested to make a $30 donation to the Forbin Project, P.O. Box 702, Cedar Falls, Iowa 50613. If you already have the program, you pay $30 for registration. If you do not have a current version of the program, you pay $40 for registration and a new disk. If you pay $50, you receive a printed manual along with registration and a disk. Currently, the 3.5-inch disk format costs $10 extra.

So much for MCI Mail. How about BITNET? I am chairman of the Electronic Mail Task Force of the chemical engineering not-for-profit educational organization, CACHE. The objective of this task force is to promote electronic mail communication among chemical engineering faculty. Presently, approximately 20% to 25% of all chemical engineering educations in the United States have their BITNET userids included in a "nicknames" list file, called RONY NAMES A0, that is suitable for use on IBM mainframes. The problem with BITNET is that it is, by original charter, limited primarily to educational users, which means universities, government research laboratories, and a few corporations. BITNET communication is the answer to e-mail communication among faculty, and has gathered considerable momentum within chemical engineering departments during the past twelve months. If you are in industry and are active, for example, in AIChE programming activities, it would be useful for you to obtain access to a BITNET node. The easiest way to do this is to pursue contacts with a chemical engineering department at a local university that already is on BITNET. Arrange for your own BITNET userid and obtain a dial-in phone number so that you can use your own modem to communicate with the university mainframe. This is, in fact, what I currently do: I create and read my BITNET messages at home, and send them over a local phone line (at 1200 baud) to the Virginia Tech mainframe.

It would be very useful for AIChE headquarters to also have access to a BITNET node. They need not become a node, just obtain access to one. I strongly recommend such an action.

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Awards

Professor J. D. Seader Wins the 1988 CAST Division Computing in Chemical Engineering Award

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

The winner for 1988 was Professor J. D. (Bob) Seader (Professor of Chemical Engineering at the University of Utah) for "his leadership in bringing FLOWTRAN from Monsanto to academia and for his many contributions in simulation, physical property correlations and databases." Professor Seader delivered his award address at the CAST Division Award Dinner on November 30, 1988, at the Washington Annual AIChE Meeting.

The supporting statement for the award reads as follows:

Bob Seader's award is for a large number of contributions to the field of computation in chemical engineering. One of his major contributions has been the Chao-Seader correlation for extrapolation of vapour pressure data into the critical region. This contribution has made practical one of the first physical property databases and steady state simulators for the analysis of gas plants that operate in a critical region. Bob also was one of the founding members of CACHE and for many years Chairman of its Large Scale System Task Force. In this capacity, the FLOWTRAN package from Monsanto was provided for use in university teaching. Books and manuals illustrating the use of FLOWTRAN for simulation purposes have been a major part of the success of this activity. Bob has continued throughout his career to make major contributions in the use of computing techniques in chemical engineering. It culminated with the recognition in 1983 when Bob delivered the AIChE Institute Lecture on "Computer Modelling of Chemical Processes". Overall, Bob has been an extraordinary contributor in the entire field of computers and chemical engineering.

Some statements for the award nomination read as follows:

"Bob Seader's contributions to the growth and excitement of our field have been numerous, varied, and often important advances that have been beneficial to large numbers of practitioners, educators, and students. His is a record of sustained achievement, with many notable landmarks.

"One of Bob's first major contributions has become known as the Chao-Seader correlation. This correlation provided one of the first quantitative bases for the extrapolation of vapor pressure data into the critical region. It permitted a generalization of the pure liquid fugacity that made it practical to build the first physical property data bases (e.g., in FLOWTRAN) and steady-state simulators for the analysis of gas plants that operate in the critical region. This was the work of a design-oriented, young chemical engineer, who thrived upon solving many vapor-liquid separation problems, while looking for generalizations and methodologies to automate the design procedure. This thirst to solve varied and new design problems has continued unabated and has resulted in several contributions of even greater significance as his orientation has matured with experience.

"By 1967, Bob had returned to academia. Bent on teaching the newest approaches to process design, and as one of the most popular and award-

winning professors at the University of Utah, Bob set out to develop or obtain for his students the best tools for Computer-aided design. He was a founding-member of CACHE and for many years Chairman of its Large Scale Systems Task Force (currently the Process Engineering Task Force). Under his leadership, FLOWTRAN was provided for usage at the universities. Our book, **FLOWTRAN Simulation – An Introduction**, was written and has subsequently sold in excess of 10,000 copies. Well over 1,000 persons, principally industrial practitioners, have taken our short-courses and learned the simulation approach to design synthesis. FLOWTRAN has been installed on the computers of over 150 Departments of Chemical Engineering and Bob played the important role of coordinating the preparation of load modules for well over 30 operating systems.

"Throughout these years, Bob solved an increasing number of design-oriented problems, which resulted first in an outstanding monograph entitled *Thermodynamic Efficiency of Chemical Processes*. This monograph, distributed by MIT Press, states in the clearest terms the principles of thermodynamic efficiency and lost work. It teaches students and practitioners how to apply the second law of thermodynamics for the design of energy-efficient chemical plants. The monograph was published during the height of the "energy crisis" and was very well-received at that time. The methodologies were eventually programmed for the DESIGN II and PROCESS simulators.

"Throughout this period, Bob continued to work on methods for simulating multi-staged towers. Many problems and brief sets of notes gave way to chapters and eventually an outstanding textbook was coauthored with Prof. Ernest J. Henley entitled **Equilibrium-Stage Separation Operations in Chemical Engineering**. This successful book has been adopted by over one-third of the faculty that teach the separations course. It is noted for its clarity and many excellent examples.

"Bob has advised numerous PhD and MS projects and, together with his students, has published many research advances throughout his career (including his 14 years in industry). In the 1970s, his papers on the synthesis of separation trains with Rodrigez and Gomez were forerunners to the flurry of activity devoted to process synthesis. He coauthored an important visionary article entitled "Synthesis in the Design of Chemical Processes" with Hendry and Rudd. His papers with deNevers were significant in clarifying the second-law analysis and were applied eventually to the efficient synthesis of thermally-coupled distillation systems. This led to the outstanding papers by Wayburn and Seader on the homotopy-continuation methods which have identified a multiplicity of steady-states in operating these towers. These, and many of the other papers written throughout his career, have stimulated researchers to further extend the ideas introduced in Bob's work.

"In 1983, Bob's excellence was recognized by the AIChE National Program Committee, who selected him to deliver the Institute Lecture at the Diamond Jubilee Meeting in Washington. Bob's lecture was one of the best in recent years and was well-received by nearly 500 persons in attendance. Subsequently, Bob wrote a monograph entitled "Computer Modeling of Chemical Processes" that expands upon his lecture. The monograph has been distributed by the AIChE.

"In further recognition of Bob's achievements, he was recently appointed as one of the three associate editors for the new **IEC Research** journal. With the advice of numerous reviewers, Bob selects the papers to be published in the design and development areas.

"Throughout his technical career, Bob has found the time to serve his Department and profession administratively." He served his Department as Chairman for three years, served the CACHE Corporation as its Executive Officer for four years, and was elected to a three-year term as a Director of the AIChE.

"Bob's illustrious career has been characterized throughout by his fun-loving, problem-solving, and enthusiastic demeanor. He is constantly questioning and challenging himself and others to excel. This has been the secret to his success as a researcher, teacher, and administrator. He is extremely deserving of the Computers in Chemical Engineering Award and I hope the Awards Committee shares our view."

Dr. C. R. Cutler Receives the 1988 CAST Division Computing Practice Award

The Computing Practice Award is intended to honor an outstanding effort that resulted in a specific embodiment, or possibly an industrial or commercial application, of computing and systems technology. The award consists of $1000 and a plaque. It was presented at the CAST Division Award Dinner, November 30, 1988, AIChE Meeting.

The winner for 1988 was Dr. C. (Charlie) R. Cutler, President of Dynamic Matrix Control Corporation for "the development and successful application of Dynamic Matrix Control technology has significantly benefited both the industrial and academic process control communities."

The award nomination statement of qualifications reads as follows:

Charlie Cutler's development and successful industrial application of Dynamic Matrix Control technology over the past seventeen years are ample reasons for his receiving the AIChE CAST Computer Industrial Practice Award. Charlie Cutler has drawn on his twenty-six years of process industry experience to refine DMC into a comprehensive process control tool consisting of a multivariable dynamic model identifier and a true constrained multivariable controller. While many types of model based controllers have been proposed and published in the academic and industrial communities, DMC has been successfully applied to a wide range of real industrial control problems. These DMC applications have resulted in substantial economic benefits for the operating companies. These economic benefits result from operating their processes at multiple constraints through the use of DMC. The DMC algorithm removes the slack normally associated with process operation under any other control technique. Charlie Cutler's success with DMC has played a major role in creating a heightened awareness in the process industries of the economic benefits associated with advanced process control. This awareness has lead to increased funding of process control research and development which benefits both the academic and industrial communities.

Dr. S. Vankataraman is the Recipient of the 1988 CAST Division Ted Peterson Student Paper Award

The Ted Peterson Student Paper Award is given to recognize an outstanding published work, performed by a student, in the application of computing and systems technology to chemical engineering. This award, supported by ChemShare and IBM, consists of $500 and a plaque. The Award will be presented on November 30, 1988 at the CAST Division Award Dinner.

The winner for 1988 is Dr. S. Vankataraman, formerly a graduate student at Clarkson University, who now works for ASPEN Tech in Boston. The award is "for his paper entitled, "Exploiting the Gibbs-Duhem Equation in Separation Calculations."

The award nomination statement of qualifications reads as follows:

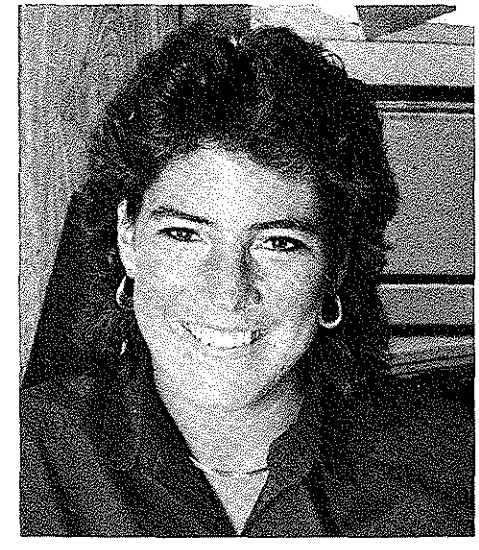
Dr. S. Vankataraman is acknowledged for his paper entitled "Exploiting the Gibbs-Duhem Equation in Separation Calculations", which was coauthored by himself and his supervisor Professor Angelo Lucia. The paper represents the first of three papers Dr. Vankataraman produced while pursuing his Ph.D. Degree in Chemical Engineering. This citation has been chosen because it represents a comprehensive treatment of the foundational ideas on which both the Ph.D. Thesis and the other two publications are based. Dr. Vankataraman was completely responsible for the development of both the conceptual ideas and the associated computer software surrounding the use of the Gibbs-Duhem equation in a Newton-like method for solving separation process models. The main ideas of the paper are rigorous and fundamentally sound from a thermodynamic and equation solving perspective. At the same time, they are of significant practical importance. They represent a monumental step in theoretical and practical aspects of equation solving techniques as they apply to the computer and systems technology and chemical engineering.

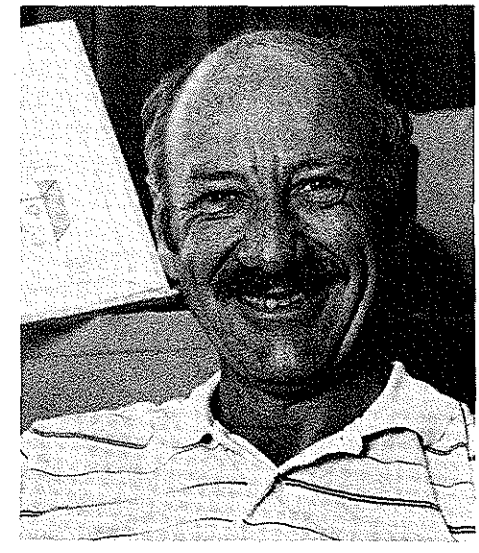
1989 CAST Division Awards Solicitation of Nominations

Please use the form on the two pages at the end of this issue to submit your nomination for the 1989 Computing in Chemical Engineering Award, 1989 Computing Practice Award, and 1989 Ted Peterson Student Paper Award. Eight copies of the nominations for the Computing in Chemical Engineering and Computing Practice Awards, and four copies of the nomination for the Ted Peterson Award, should be sent by April 3, 1989 to Professor G.V. (Rex) Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907 (317) 494-4089.

SimuSolv*: A Computer Program For Building Mathematical Models

by Kay E. Kuenker and Gary E. Blau, Global Ag Math Modeling & Analysis Agricultural Chemical Process Research, Dow Chemical Company, Midland, Michigan





Introduction

Developing mathematical models of physical and chemical systems is a fundamental part of learning how processes work. Building such models is iterative, as shown in Figure 1. Data are collected and models are proposed to correlate and explain the data. When necessary, more data are collected and additional hypotheses are made until a validated model is obtained. One of the characteristics of these mathematical models is their inherent nonlinearity in the model parameters. As a result, the use of standard statistical tools such as linear regression analysis[1] are not valid for the parameter estimation or "fitting" portion of the model building exercise. Although the theoretical aspects of the nonlinear parameter estimation problem had been documented[2], user-friendly software was not available within the Dow Chemical Company to perform this important task. Consequently, the building of nonlinear models for reaction kinetics, pharmacokinetics, or ecokinetic systems became the domain of "professional" model builders, that is, scientists and engineers with a strong programming background (frequently referred to as computer jocks), a working knowledge of nonlinear statistical principles, and some knowledge of the physical systems involved.

In the late seventies, it became apparent to Dow management that a significant impact on the profitability of Dow processes and products could be realized by better understanding how they worked. This stimulated the need to build mathematical models by researchers throughout the organization and not just by the "chosen few". Funds were provided to a corporate organization to develop a state-of-the-art piece of software that could be used by the nonprofessional modeling community in Dow. The mission was to allow a user with a minimal working knowledge of

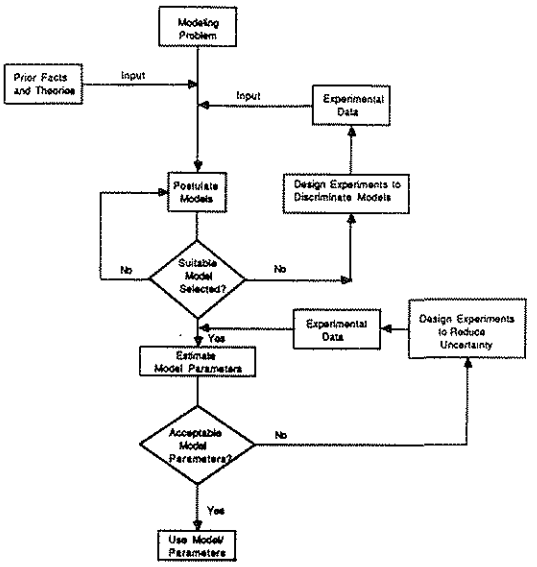


Figure 1. The Iterative Process of Model Building

calculus, nonlinear parameter estimation techniques, optimization theory, and computer science, but a good physical understanding of the fundamental process involved, the ability to use the software to build and validate meaningful mathematical models.

The results of this effort was a program called DACSL[3]. It was used extensively throughout the company for its intended purposes. As knowledge of its existence became known, vendors approached Dow about marketing the product outside of the company. In 1985, Gary Blau and Doug Leng helped create a new Engineering Research Laboratory in Dow's Central Research Organization. The charter of the organization was to build new businesses in new technology areas for Dow. In 1986, Bob Nowak, director of the Central Research Laboratories, asked Gary to investigate the possibility of marketing SimuSolv outside of Dow. With the success of DACSL internally and a strong interest from various governmental and industrial beta test sites, Dow decided to launch a software business. Gary Agin, the engineer who had developed the original DACSL program was brought in and Jake Eichhorn, a technical business manager, was identified. Kay Kuenker, the coauthor of this paper joined the team coincidentally with the product launch in 1987. At the time of this writing, SimuSolv is being used by chemical engineering departments in several major universities, by governmental agencies, and by industries in a variety of application areas. The remainder of this paper gives a global overview of the capabilities of the product in the application areas of chemical engineering and nonlinear experimental design. Please refer to the bibliography for sources describing other primary application areas in which SimuSolv has been used[4,5,6].

Overview

The SimuSolv* computer program is an integrated, multifunctional, software package that is useful in each stage of the model building process. It is designed to simulate dynamic physical systems, to estimate parameter values that best fit models to observed data, and to optimize complex nonlinear models. Fundamental to the program's operation is its ability to solve systems of ordinary differential equations that describe the dynamic behavior of the physical systems involved. During a simulation, SimuSolv automatically integrates the differential equations in the math model without requiring the user to become an expert in numerical methods. A variety of integration methods are available to suit the needs of the particular model. These range from simple fixed-step methods to stiff-equation solvers, including the LSODE code developed by A.C. Hindemarsh (1980)[7].

For optimization and parameter estimation, SimuSolv currently provides two methods. The first is an extension of the direct-search method originally developed by Spendley, et al. in 1962[8], which is particularly

useful for problems with only a few adjustable parameters to optimize or estimate. The second is the generalized reduced gradient method (GRG2) developed by Lasdon, et al. in 1978[9], which is effective for larger problems. The latter method has been enhanced by the addition of the direct decoupled method (DDM), one of the most efficient and robust sensitivity analysis procedures available[10]. DDM uses gradients of the objective function already calculated by GRG2 and hence does not add greatly to the computational burden[11]. Details about specific integration and optimization algorithms are discussed in Blau et al[3]. In the future versions of SimuSolv, a Marquardt method and Sequential Quadratic Programming methods are anticipated.

I The Language of SimuSolv

The language of SimuSolv is really a combination of two languages having unique functions. The first is ACSL**, The Advanced Continuous Simulation Language[13], which is used to write the model definition program, and the second is the Run-Time Command Language which is used in communicating with the executive. These languages are high-level in the sense that they allow the user to accomplish many types of complicated computational tasks with a minimal amount of computer programming. Whenever possible, there are defaults provided that are generally appropriate. The user can concentrate on the modeling task itself, rather than spending unnecessary time on the computational methodology. The terms used in the language have been chosen to be meaningful and mnemonic in order to facilitate the learning process. Although the language of SimuSolv is designed to be easy to learn and use, the power and versatility of the underlying computational and numerical analysis methods have not been compromised to achieve that end. For the more sophisticated user, error bounds, integration methods and step size, and other characteristics of the computations are user controlled if desired. Macro facilities are a part of the language and FORTRAN subroutines can be incorporated into the program to tailor it to special needs. Before SimuSolv can be invoked, a model definition program must be written in ACSL. The program generally consists of the following three distinct segments:

INITIAL: The code in this segment is executed at the beginning of each simulation. Initial values are assigned to variables and preliminary calculations are performed.

DYNAMIC: This segment defines the dynamic or time varying aspects of the model. All the differential equations are placed here along with other statements that are required during the course of a simulation.

TERMINAL: The code in this segment is executed only at the end of a simulation.

In addition to a model definition program, a run-time command file is needed. This file contains any experimental data to be analyzed such as for parameter estimation. The data are entered into the file in a familiar table format with the column headings being model variable names. These column headings are used for both parameter estimation and graphical comparison of calculated and observed values.

There are two phases in the use of SimuSolv. In the first phase the model of the physical system, written in the ACSL language, is translated into FORTRAN, compiled, linked with SimuSolv subroutines and any subroutines the user wishes to include, creating an executable computer module with which the user interacts. In the second phase, the user enters into a dialogue with SimuSolv, during which he or she controls the activities of the program. The user may ask for simulation, parameter estimation, optimization, graphs or tables of results, and so on. Provision is made for hardcopy documentation.

II How Has SimuSolv Been Used?

Chemists and engineers use SimuSolv extensively to develop the mathematical models required for the effective design, debottlenecking and optimization of chemical processes. It is employed in research to model the kinetics of reacting systems, in engineering to model reactors and other unit operations, and in production to help optimize entire processes. Models of unit operations have been incorporated into steady-state simulation programs such as ASPEN* and PROCESS**, making SimuSolv a valuable complement to these large programs. The dynamic nature of the models makes them very useful in studying start-up and control strategies for coupled unit operations.

The SimuSolv program is ideally suited to modeling the operation of a chemical reactor, the key unit operation in any chemical process[13]. Batch or well-mixed flow reactors can be simulated in a straightforward manner by sets of ordinary differential equations. Fixed-bed reactors, for which both dynamic and spatial effects must be considered, are simulated by sets of partial differential equations. These equations are decomposed in SimuSolv into arrays of ordinary differential equations for easy, efficient handling. A reactor model must contain a verified model of the reaction kinetics. SimuSolv is used effectively to build such kinetic models. SimuSolv has been incorporated as an integral part of the iterative procedure, which was shown in Figure 1. Starting with available data and some knowledge of the chemical reactions, one or more kinetic models are postulated. These

conceptual models are translated into a model definition program and SimuSolv is then used to compare calculated and experimental results. The models and the data are studied to determine where the data or kinetic models are inadequate. Quite frequently, additional experiments must be designed to distinguish between the models or to get good estimates of model parameters. The parameter estimation features of SimuSolv are invoked to obtain the best set of kinetic parameters for each proposed model and, finally, the statistical output from SimuSolv is examined to help decide which model is the best one. This procedure leads to a kinetic model that can be incorporated with confidence into an engineering model of a reactor. To illustrate the capabilities of SimuSolv as well as the concepts of modeling and design of experiments for model discrimination and parameter estimation, several examples will be presented.

III Parameter Estimation With SimuSolv

Consider the following chemical model:

$$EO + NH3 \xrightarrow{K_1} MEA$$

$$EO + MEA \xrightarrow{K_2} DEA$$

$$EO + DEA \xrightarrow{K_3} TEA$$

where

EO = ethylene oxide
NH3 = ammonia
MEA = mono-ethanolamine
DEA = di-ethanolamine
TEA = tri-ethanolamine

and the corresponding kinetic model

$$dMEA/dt = K_1*EO*NH3 - K_2*EO*MEA$$
$$dDEA/dt = K_2*EO*MEA - K_3*DEA*EO$$
$$dTEA/dt = K_3*EO*DEA$$
$$EO = EOIC-(MEA-MEAIC)-2(DEA-DEAIC)-3(TEA-TEAIC)$$
$$NH3 = NH3IC-(MEA-MEAIC)-(DEA-DEAIC)-(TEA-TEAIC)$$

The following Table shows the available set of sequential-concentration data, as a function of time, for components MEA, DEA, and TEA:

DATA

Time	MEA	DEA	TEA
0.0	0.0	0.0	0.0
0.1	0.39	0.09	0.01
0.2	0.46	0.20	0.03
0.3	0.43	0.31	0.10
0.4	0.37	0.37	0.15
0.8	0.34	0.39	0.19
1.0	0.32	0.40	0.22
1.2	0.29	0.40	0.25
1.4	0.28	0.40	0.26
1.6	0.27	0.41	0.28
1.8	0.27	0.42	0.28
2.0	0.25	0.42	0.29

END

Questions that need to be answered are:

1. What are the best values for the rate constants K_1, K_2, and K_3?
2. What are the standard deviations or uncertainties in these estimated rate constants?
3. How well do the calculated curves fit the data?

The first step to be taken in order to answer these questions is to translate the kinetic model into a SimuSolv model definition program in the ACSL language. Every model definition program follows the same format, beginning with the word PROGRAM and ending with the word END. In between are the three optional segments, *INITIAL*, defining the initial conditions, *DYNAMIC*, containing the time varying portions of the model, and *TERMINAL*, which performs calculations after integration has been completed. A model definition program of the above process is shown below.

The dollar ($) sign allows one to place more than one statement on a line, comments are placed between single quotes, and the ellipses (...), permit the continuation of one line to the succeeding one.

The second step is to invoke SimuSolv and get into the run-time mode. To perform a simulation, i.e., solve the differential equations, a **START** command is used. A graphical display of the results of the simulation is obtained with the command **PLOT** MEA DEA TEA.

Figure 2 shows that the values calculated by the model follow the basic shape of the data. However, the rate constants K_1, K_2, and K_3 are not at their optimal values to yield the best fit. SimuSolv allows the user to interact with the model to study the effect of changing the values of K_1, K_2, and K_3. This interaction allows the user to more fully understand the sensitivity of the model to parameter changes. Once the best "eye-fit" to data is obtained, SimuSolv can be used to estimate the optimum values for the parameters K_1, K_2, and K_3.

SimuSolv uses the method of maximum likelihood to perform parameter estimation[2]. This method maximizes the probability that a particular set of parameter estimates, e.g., K_1*, K_2*, K_3*, generated the experimental data. The generation of maximum likelihood estimates is an iterative process. Starting with initial guesses of the parameters supplied by the user, nonlinear optimization techniques are used to generate successive values of the parameters which are selected to maximize a likelihood function. This likelihood function is the calculated probability of our having measured a given set of data given the current set of parameters and the correct model. Another attractive feature of the method of maximum likelihood is the ability to estimate the parameters of a statistical model of experimental error variability along with the parameters of the mathematical model. This

statistical model is used to properly weight the data extracting the greatest information content from those data points that have the smallest variability. One restriction, however, is that the form of the error model must be assumed a priority. In SimuSolv, these assumptions take the following form:

1. The experimental errors are normally distributed.
2. The measured values are independent of each other (the validity of this assumption is questionable even though the experimentalist generally strives to make it true for his or her measurements).
3. The measured values are uncorrelated.

The final assumption is unique to SimuSolv and requires some explanation. The variability of the measured values is given by the relationship,

$$\sigma ij^2 = \omega ij^2 f_i^{\gamma_i}(\underline{\theta}, t_j)$$

where

σij^2 is the variance of the i^{th} response for the j^{th} data point t_j (for simplicity, it will be assumed that time is the only independent variable).

$f_i(\underline{\theta}, t_j)$ is the predicted values of the i^{th} response for the j^{th} data point

ωij^2 is a statistical parameter

γ_i is another statistical parameter called the heteroscedastisity parameter.

This functional form simply relates the variability of the measurement to the magnitude of the measured values. Two limiting cases are of interest. When $\gamma^i = 0$, $\sigma_{ij}^2 = \omega_{ij}^2$ so the variability is *constant* over the entire data region. When $\gamma^i = 2$, the variability is directly proportional to the measured values. This latter case corresponds to the situation where the relative errors in the measurements are constant over the experimental region. In SimuSolv, the parameters ω_{ij} and γ_i are estimated along with the parameters of the mathematical model (K_1, K_2, and K_3 in this example). This

```
PROGRAM
    INITIAL
        Variable      Time = 0.0                          $'Define Run variable'
        Constant      K1 = 3.0, K2 = 2.0, K3 = 1.0        $'Initial Parameter Estimates'
        Constant      NH3IC = 1.0, EOIC = 3.0             $'Starting Material'
        Constant      MEAIC = 0.0                         $'Initial values for'
        Constant      DEAIC = 0.0                         $'State variables'
        Constant      TEAIC = 0.0
        Constant      TSTOP = 2.0                         $'Length of experiment'
        CINTERVAL     CINT = TSTOP/50.                    $'Communication interval'
    END
        DYNAMIC
            DERIVATIVE
                      'Write differential equations'

                      DMEADT    = K1 * EO * NH3 - K2 * EO * MEA
                      DDEADT    = K2 * EO * MEA - K3 * EO * DEA
                      DTEADT    = K3 * EO * DEA

                      'Integrate Differential Equations'

                      MEA       = INTEG(DMEADT,MEAIC)
                      DEA       = INTEG(DDEADT,DEAIC)
                      TEA       = INTEG(DTEADT,TEAIC)

                      'Write Mass Balances'

                      EO        = EOIC - (MEA - MEAIC) - 2*(DEA - DEAIC) - 3*(TEA - TEAIC)
                      NH3       = NH3IC - (MEA - MEAIC) - (DEA - DEAIC) - (TEA - TEAIC)
            END
        TERMT(TIME .GE. TSTOP)  $'Test to Determine End of Integration'
    END
    TERMINAL
    END
END
```

GRAPHICAL SIMULATION OUTPUT

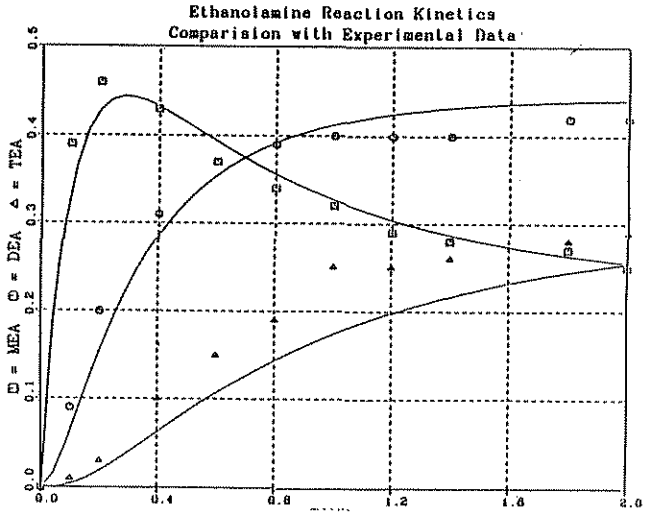


Figure 2: Graphical Output of Comparison of Reaction Kinetics with Experimental Data

GRAPHICAL OUTPUT AFTER OPTIMIZATION

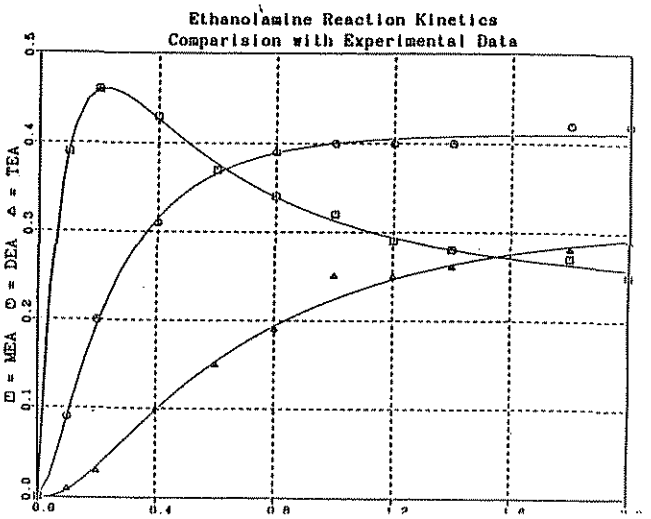


Figure 3: Graphical Output After Parameter Estimation. Comparison of Reaction Kinetics with Experimental Data.

assures that the data are properly weighted in a statistical sense. The user can control the weighting, but a properly designed experiment with replication is preferred. To obtain the likelihood estimates in the example problem, the following commands are issued:

VARY $K_1 K_2 K_3$
FIT *MEA DEA TEA*
OPTIMIZE

The resulting plot is shown in Figure 3.

When SimuSolv has found the likelihood estimators, it does one final simulation to prepare a set of calculated values for graphing, and then it reports the results of the estimation process (see Table 1). There is a lot of statistical information in the report, but this discussion will focus on just a few of the items. Under PARAMETER ESTIMATES, the initial and final values of the rate constants are presented with an improvement (increase) in the Likelihood Function. *STANDARD DEVIATION* gives a measure of the uncertainty in the estimates of the rate constants. The *OBSERVED* and *PREDICTED* values of the three variables are self explanatory. *RESIDUAL PLOTs* are bar graphs showing in an approximate manner how the *RESIDUALS* are distributed. Other parts of the report are discussed in more detail in the SimuSolv Introductory Guide[14].

SimuSolv also can help us answer questions of uncertainty or quality of the parameter estimates. Contour plotting features allow one to graphically view the confidence regions for the estimated parameters. There are three methods for calculating these regions: (1) Linear, which is based on a Taylor series approximation, (2) Nonlinear, which uses the F-statistic[15], and (3) Exact, which is based on Bayes' Theorem[16]. These confidence regions can be obtained by using the MAP command in SimuSolv (Figure 4).

In addition to confidence regions, two- and three-dimensional graphics of the objective function may be obtained by using various subcommands of the **MAP** command. The surface plot of the Log Likelihood Function is shown in Figure 5.

IV Nonlinear Experimental Design with SimuSolv

During the model building process, it is frequently possible to postulate several physically meaningful mechanistic models to represent the process under study. The problem is to discriminate or choose between these postulated models using statistical analysis until the most suitable one is found. At times, however, the information content of the data is so low that it is impossible to discriminate between models. Therefore, additional experiments need to be designed. SimuSolv is a very useful tool for this purpose. It can be used to determine where in an operating region the postulated models predict different results from one another. Such points are the most useful for discriminating rival models. The following example will illustrate these concepts.

Consider the following gaseous reaction for the reduction of nitric oxide[17]:

$$NO + H_2 \xrightarrow{or} H_2O + \tfrac{1}{2}N$$
$$A + B \xrightarrow{or} C + \tfrac{1}{2}D$$

The reaction was conducted in a differential reactor over a commercial solid catalyst consisting of copper, chromia, and zinc. Experimental conditions were maintained such that the reverse reaction did not take place to any appreciable extent. Experimental data were gathered by running the experiments such that the partial pressure of A was held constant at 0.05 atm while the partial pressure of B was varied from 0.009 to 0.05 atmospheres, and vice versa. This one-at-a-time experimentation scheme was run at three different temperatures, and the reaction rate was measured and recorded for each run. Based on the plots of the data, the experimenters suspected that a surface reaction was controlling. Consequently, they postulated the following three plausible mechanistic models:

Model 1: Reaction between one adsorbed A molecule and one gaseous molecule of B:

$$r = \frac{kK_A P_A P_B}{(1 + K_A P_A + K_B P_B)} \qquad \text{(Model 1)}$$

Model 2: Reaction between one adsorbed B molecule and one gaseous molecule of A:

$$r = \frac{kK_B P_A P_B}{(1 + K_A P_A + K_B P_B)} \qquad \text{(Model 2)}$$

Model 3: Reaction on surface between two adsorbed molecules of A and B:

$$r = \frac{kK_A K_B P_A P_B}{(1 + K_A P_A + K_B P_B)^2} \qquad \text{(Model 3)}$$

All three model equations are of the form:

$$y_i = f(\underline{x}_i, \underline{\theta}) + \varepsilon_i \quad i = 1, \ldots, n$$

where

- y = r response variable
- $\underline{x}$ = (P_A, P_B, T) independent variables
- $\underline{\theta}$ = (k, K_A, K_B) parameters
- i = i^{th} data point
- n = number of data points
- ε_i represents the experimental error in the i^{th} data point.

It was assumed that the kinetic rate constant k exhibited the familiar Arrhenius temperature dependence:

$$k = k^{\circ} \exp\left(\frac{-E}{RT}\right).$$

where k° is a pre-exponential factor and E is the activation energy. The adsorption coefficients, K_A and K_B, were felt to be constant over the temperature range. The nonlinear

```
                                DESCRIPTION    PARAMETER ESTIMATES      STANDARD
                                -----------    -------------------      DEVIATION
                                               INITIAL      FINAL
                    LOG LIKELIHOOD FUNCTION     81.804      146.13
                                         K1     3.0000      4.0244     6.845E-02
                                         K2     2.0000      2.4710     2.484E-02
                                         K3     1.0000      1.4860     1.770E-02

                MEA          MEA                      STANDARDIZED   RESIDUAL
  TIME      OBSERVED     PREDICTED        % ERROR      RESIDUAL        PLOT

0.0000E+00 0.0000E+00 0.0000E+00          0.00      0.000E+00          |
0.1000      0.3900      0.3921          -0.54       -0.466           *|
0.2000      0.4600      0.4587           0.27        0.279           |**
0.4000      0.4300      0.4268           0.73        0.704           |***
0.6000      0.3700      0.3768          -1.85        -1.52       *****|
0.8000      0.3400      0.3391           0.28        0.209           |*
 1.000      0.3200      0.3123           2.40         1.71           |********
 1.200      0.2900      0.2934          -1.17       -0.759        ***|
 1.400      0.2800      0.2798           0.06      3.783E-02         |*
 1.600      0.2700      0.2700           0.01      5.306E-03         |
 1.800      0.2700      0.2627           2.69         1.62           |*******
 2.000      0.2500      0.2574          -2.95        -1.65       *****|

                DEA          DEA                      STANDARDIZED   RESIDUAL
  TIME      OBSERVED     PREDICTED        % ERROR      RESIDUAL        PLOT

0.0000E+00 0.0000E+00 0.0000E+00          0.00      0.000E+00          |
0.1000     9.0000E-02 8.9468E-02          0.59          0.201        |*
0.2000      0.2000      0.1944           2.81           1.43        |******
0.4000      0.3100      0.3150          -1.60          -1.01       ****|
0.6000      0.3700      0.3668           0.87          0.605         |***
0.8000      0.3900      0.3901          -0.03      -2.154E-02         |
 1.000      0.4000      0.4012          -0.30          -0.219        *|
 1.200      0.4000      0.4067          -1.67          -1.20      *****|
 1.400      0.4000      0.4095          -2.36          -1.68      ******|
 1.600      0.4100      0.4109          -0.21          -0.152        *|
 1.800      0.4200      0.4116           2.01           1.48        |*******
 2.000      0.4200      0.4119           1.93           1.42        |******

                TEA          TEA                      STANDARDIZED   RESIDUAL
  TIME      OBSERVED     PREDICTED        % ERROR      RESIDUAL        PLOT

0.0000E+00 0.0000E+00 0.0000E+00          0.00      0.000E+00          |
0.1000     1.0000E-02 8.3025E-03         16.98          0.600        |***
0.2000     3.0000E-02 3.3901E-02        -13.00          -1.32       ****|
0.4000      0.1000     9.7458E-02          2.54          0.832        |****
0.6000      0.1500      0.1517          -1.16         -0.559         **|
0.8000      0.1900      0.1927          -1.42         -0.866        ***|
 1.000      0.2200      0.2229          -1.33         -0.929       ****|
 1.200      0.2500      0.2452           1.93           1.53        |*******
 1.400      0.2600      0.2617          -0.64         -0.523         **|
 1.600      0.2800      0.2739           2.17           1.92        |*********
 1.800      0.2800      0.2831          -1.11         -0.980       ****|
 2.000      0.2900      0.2900           0.00      -1.609E-03         |
```

STATISTICAL SUMMARY

	MAXIMIZED LOG LIKELIHOOD FUNCTION	WT RESID SUM OF SQUARES	WEIGHTED RESIDUAL SUM	STANDARD ERROR OF ESTIMATE	PERCENTAGE VARIATION EXPLAINED	WEIGHTING PARAMETER
OVERALL	146.1	1.293E-03	2.070E-02		99.883	
MEA	47.86	2.411E-04	7.580E-04	5.175E-03	99.841	0.00
DEA	46.01	9.207E-04	2.104E-02	5.553E-03	99.885	0.99
TEA	52.26	1.308E-04	-1.104E-03	3.582E-03	99.916	0.07

CORRELATION MATRIX

	K1	K2	K3
K1	1.000		
K2	0.5503	1.000	
K3	0.5912	0.5193	1.000

VARIANCE-COVARIANCE MATRIX

	K1	K2	K3
K1	4.6853E-03		
K2	9.3563E-04	6.1698E-04	
K3	7.1615E-04	2.2829E-04	3.1322E-04

```
OPTIMIZATION METHOD: NELDER-MEAD SEARCH

SUCCESSFUL TERMINATION: STANDARD DEVIATION OF OBJECTIVE
                        FUNCTION WAS LESS THAN SDFOPT.
                        SDFOPT =  1.00000E-05

FUNCTION EVALUATIONS FOR OPTIMIZATION =  86
FUNCTION EVALUATIONS FOR STATISTICS   =  7
OPTIMIZE TIME =  10.020 SECONDS
SIMUSOLV>
```

Table 1. Statistical Output from Parameter Estimation

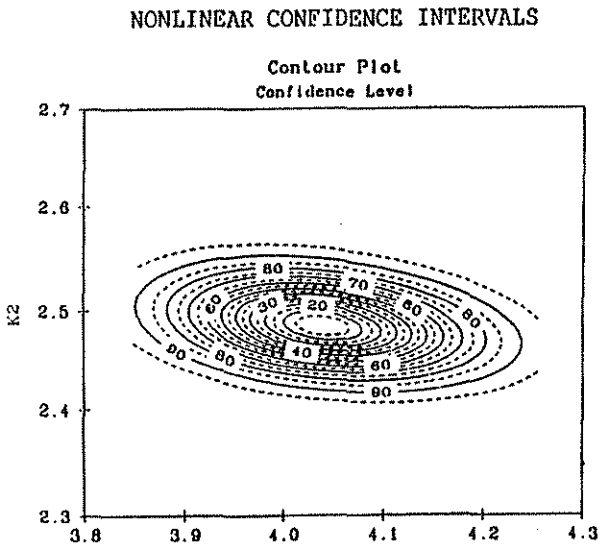


Figure 4. Nonlinear Confidence Intervals for K_1 and K_2 generated by the command **MAP** NONLIN.

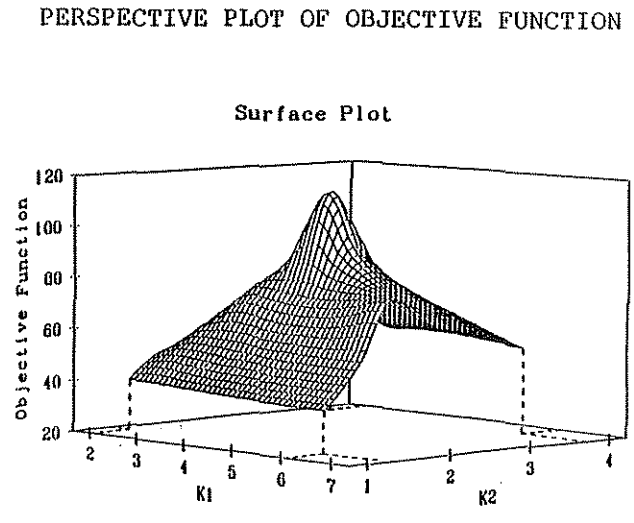


Figure 5. Three Dimensional Surface Plot of the Objective Function Used in Parameter Estimation. Generated with the Command: **MAP** FUNCTION 3-D.

parameter estimation capabilities of SimuSolv can be used to estimate the parameters θ for each of the postulated models. Table 2 shows an isothermal analysis of the data. The point estimates for the parameters are presented at the different temperatures; they suggest that Model 3 be selected over models 1 and 3 since the adsorption constants are positive for Model 3. Table 3 shows a nonisothermal analysis of the data. It is now no longer possible to reject models based on the signs of the parameters and statistical criteria such as likelihood ratios or residual analysis, which are normally used to discriminate the models. The likelihood ratios presented in Table 3 fail to discriminate Model 1 from Model 2 but suggest that Model 3 is preferred.

The three-dimensional graphics capabilities of SimuSolv were used to compare all three models over the entire experimental region. To compare the models, a difference function was set up and plotted over an extrapolated experimental region. The difference between models 1 and 3 is shown in Figure 6 and Figure 7 by a contour plot and surface plot, respectively. Examining the figures

Temp., °C	$k \times 10^4$ g-mole/(min) (g-catalyst)	K_A,atm^{-1}	K_B,atm^{-1}	Log Likelihood
		MODEL 1		
375	2.45E-3 ± 2.18E-4	3.60E5 ± 3.36E7	5.45E5 ± 5.09E7	4.59
400	3.20E-3 ± 8.31E-4	935.0 ± 1.78E4	732.142E4	-9.23
425	8.41E-3 ± 1.59E-4	2.64E5 ± 5.96E7	5.04E5 ± 1.14E8	-10.80
		MODEL 2		
375	1.60E-3 ± 1.13E-4	4.28E5 ± 6.24E7	6.49E5 ± 9.43E7	4.59
400	4.10E-3 ± 1.49E-3	1130.0 ± 2.48E4	880 ± 1.94E4	-9.20
425	4.55E-3 ± 5.38E-4	8.96E4 ± 1.23E7	1.56E5 ± 2.15E7	-10.84
		MODEL 3		
375	5.13E-4 ± 1.25E-4	13.4 ± 4.33	18.8 ± 4.52	5.08
400	4.66E-4 ± 8.05E-5	48.8 ± 20.6	47.0 ± 19.0	-4.20
425	1.02E-3 ± 3.70E-4	23.0 ± 14.9	33.7 ± 17.8	-9.7

Table 2: Isothermal Data Analysis

Parameters	Model 1	Model 2	Model 3
k°	4.75E-3 ± 1.47E-3	3.04E-3 4.13E—	4.7E-4 8.65E-5
E	19.6 ± 1.30	19.6 ± 1.27	19.8 ± 1.03
K_A	130 ± 350	207 ± 793	40.6 ± 17
K_B	199 ± 498	314 ± 1154	46.9 ± 17
Log Likelihood Function	-31.4	-30.7	-24.6

Table 3: Nonisothermal Data Analysis

on the contour plot it is evident that the models are the most different in the upper right corner where the partial pressure of A is 0.5 and that of B is 0.5. Looking at the surface plot shows the same thing, however, the vertical axis illustrates that there is really very little difference at all between Model 1 and Model 3. Figure 8 shows the surface plot of the difference between models 1 and 2 for nonisothermal data analysis with temperature versus partial pressure of A. Again the greatest difference between the models appears to be where the partial pressure of A is 0.5 and the temperature is high. Thus, to correctly discriminate among models, additional experiments should be designed and run where the models are the most different.

V Design of Experiments For Parameter Estimation

Once the model discrimination process has been completed and a suitable model found, it is necessary to find the best parameter estimates for that model. SimuSolv can be used to determine the maximum likelihood estimators of the parameters and quantify the uncertainty in the estimates. There are three methods in SimuSolv to approximate the confidence regions around the adjustable parameters: (1) Linear, (2) Nonlinear, and (3) Exact. The Linear Method gives an approximation of the confidence region by truncating at the second term of a Taylor series expansion of the function around the likelihood estimators. The second method uses the nonlinear form of the model, but employs the F-statistic to determine the confidence limits, which is valid for linear models only. The Exact method is based on Bayes' Theorem, which uses prior probabilities of the parameters and the likelihoods of those parameters[14]. If the confidence regions are unacceptable, the modeler is forced to collect additional experimental data to reduce or minimize the uncertainty in these parameter estimates. SimuSolv becomes a very useful tool for locating experimental conditions that will reduce this uncertainty since it is possible to simulate the confidence regions over the experimental regions *before* the experiments are conducted. This concept is best illustrated by example.

Consider the following reaction scheme:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Estimate k_1 and k_2 from the following sequential concentration time data and determine the uncertainty in the parameter estimates:

Time	Concentration
1.0	70.2
2.0	81.9
4.0	76.4
7.0	74.1
24.0	50.7
48.0	37.4
55.0	20.5
72.0	18.3

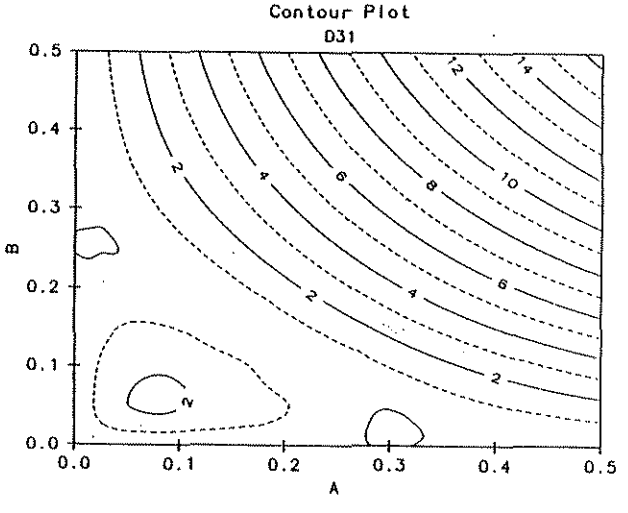


Figure 6: Contour Plot of the Objective Function: The Difference Between Model 1 and Model 3.

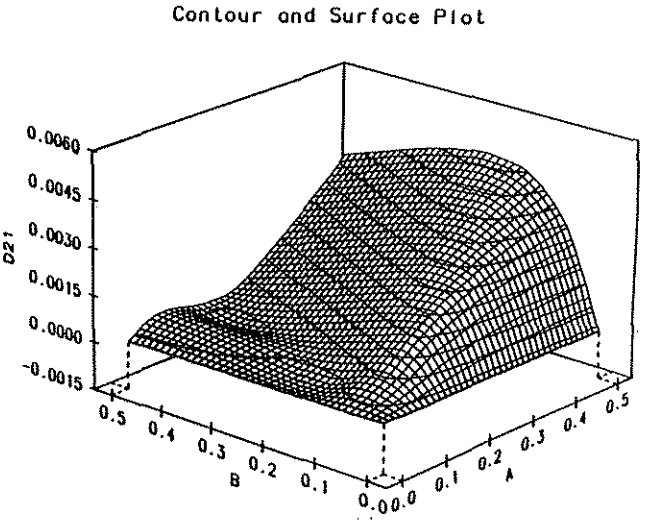


Figure 7: Surface Plot of the Objective Function: The Difference Between Model 1 and Model 3.

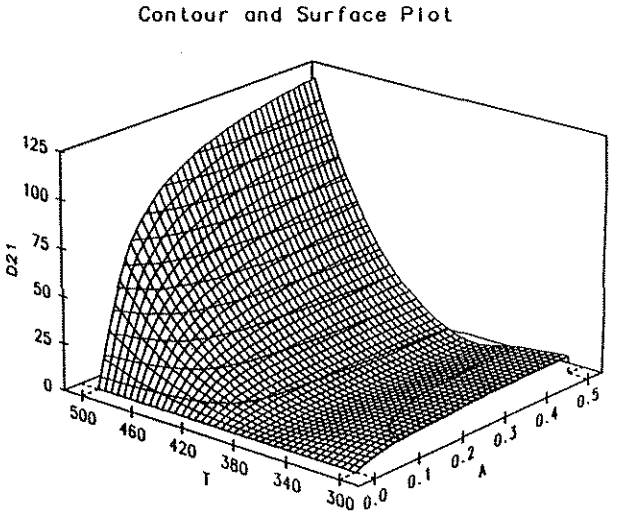


Figure 8: Surface Plot of Objective Function: The Difference Between Model 1 and Model 2 with Nonlsothermal Data Analysis

To solve this problem using SimuSolv proceed in the same manner as the other illustrations, building the ACSL model definition program, and performing simulations and parameter estimation, thereby obtaining the maximum likelihood estimators for k_1 and k_2. The graphical result of this is shown in Figure 9, which shows that the fit of the data is very reasonable. But the question must be asked, How good are those parameter estimates? or, stated in another way, What is the confidence region around k_1 and k_2?

The confidence regions calculated using the Linearization method are shown in Figure 10. This elliptical region suggests that a high degree of confidence can be placed in the fact that k_1 and k_2 are at their optimum. However, if the confidence regions are generated using the exact method, a totally different result is obtained as illustrated in Figure 11. In this figure, note that k_2 is bounded above and below by 0.028 and 0.016, respectively. Although k_1 is bounded below by 1.75, it appears to be unbounded above, implying that the area of the confidence region is infinite. The experimental data provide an explanation for this phenomenon. By referring to the fit of data from Figure 9, note that k_2 is determined from 7 data points whereas the uptake rate k_1 is determined by one point only. Therefore, it suggests additional experiments in the region of 0 to 1.0 hours. For example, by adding one additional data point taken at time = 1.0 hours and re-fitting the data, the confidence region was greatly improved, as shown in Figure 12.

VI Optimization With SimuSolv

In the previous examples, the use of SimuSolv for nonlinear parameter estimation and experimental design in the building of mechanistic models has been emphasized. However, once such models have been built and validated, SimuSolv can be used to optimize their performance. SimuSolv contains the nonlinear parameter optimization code GRG2 developed by Lasdon[9]. Any objective function and nonlinear constraints can be defined in the model definition program. Then the commands *MAXIMIZE* or *MINIMIZE* are used in the run-time environment to call this objective function. The *VARY* command demonstrated earlier is used to identify those parameters to be optimized. If the parameters are subject only to univariate constraints, a direct search method is also available. As with any nonlinear optimization procedure, the quality of the initial estimates supplied by the user are the primary factors in controlling the performance of the optimization procedures both in terms of efficiency and convergence to an optimum. One particularly attractive feature of doing optimization with SimuSolv is the ability to use the MAP command and other graphical features to display the behavior of the objective function in the vicinity of the optimum for any pair of optimization variables. This can frequently help the user avoid false optima or saddle points.

Conclusion

SimuSolv is a very useful tool for building and optimizing models characterized by systems of differential equations. It is being used extensively in academic, industrial, and governmental agencies by scientists and engineers who have a need to build and use mathematical models but who are not professional modelers. SimuSolv is available for both the IBM and DEC Mainframes as well as MICROVAX and SUN workstations. The package is being developed and enhanced by Dow Chemical Company's Engineering Research Laboratory. Some

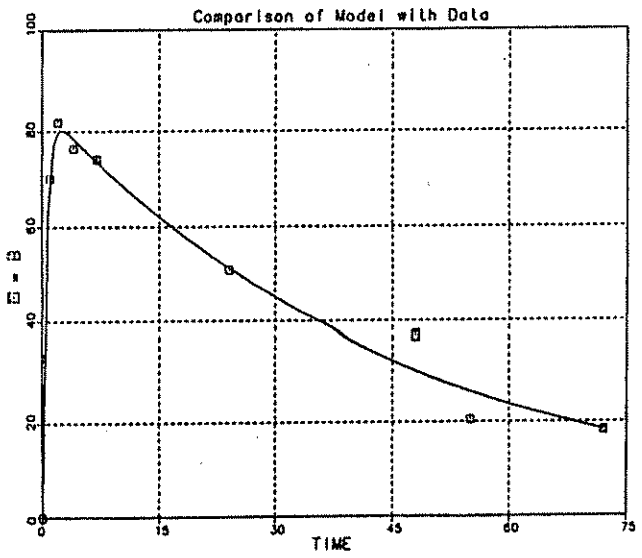


Figure 9: Graphical Output from Parameter Estimation. Comparison of Simulation Results to Experimental Data.

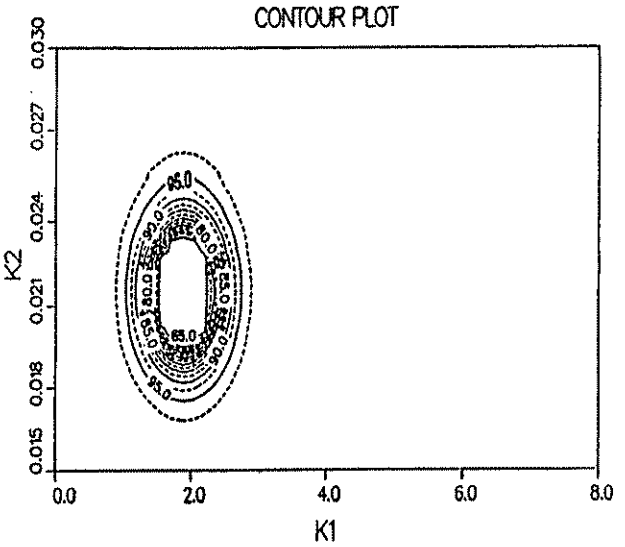


Figure 10: Confidence Regions for k_1 and k_2 Calculated by Linear Approximation.

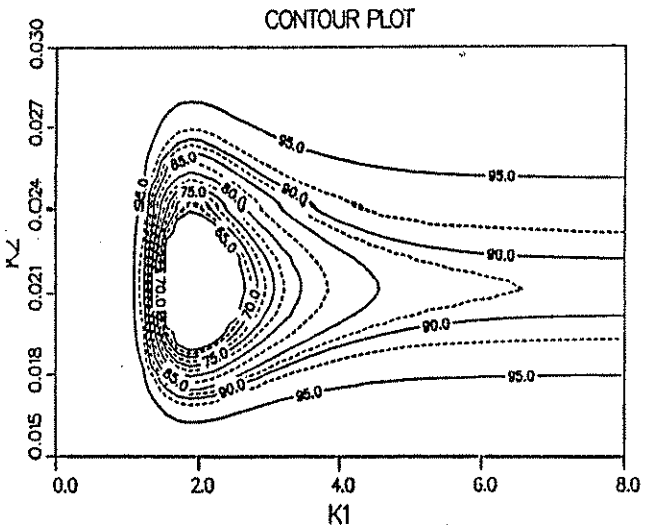


Figure 11: Confidence Regions for k_1 and k_2 Calculated Using the Exact Method.

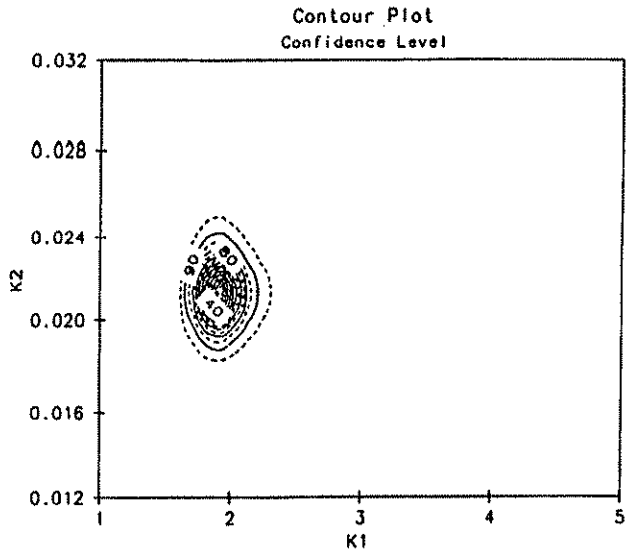


Figure 12: Confidence Regions for k_1 and k_2 Calculated Using the Exact Method with One Additional Data Point at time = 0.5 hours.

anticipated enhancements are the abilities to handle systems of algebraic and differential equations simultaneously, to design experiments for both model discrimination and parameter estimation, and to readily handle systems of partial differential equations. The product is being marketed in the United States and Canada by Mitchell and Gauthier Associates, 73 Junction Square Drive, Concord, MA, 01742, (617) 369-5115, and in Europe by Rapid Data, Inc., Brighton, England. These organizations may be contacted by individuals interested in licensing the product.

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Computer-Assisted Process and Control Engineering

by Authors: W. Westerberg, Henry Chien, James M. Douglas, Bruce A. Finlayson, Roland Keunings, Manfred Morari, Jeffrey J. Siirola, and William Silliman

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Abstract

Computers and computational methods have advanced to the point where they are beginning to have significant impact on the way in which chemical engineers can approach problems in design, control, and operations. The computer's ability to handle more complex mathematics and to permit the exhaustive solution of detailed models will allow chemical engineers to model process physics and chemistry from the molecular scale to the plant scale, to construct models that incorporate all relevant phenomena of a process, and to design, control, and optimize more on the basis of computed theoretical predictions and less on empiricism. This chapter explores the implications of these changes for process design, control, operations, and engineering information management. Future developments and opportunities in process sensors are also covered.

Imagine a room 50 feet long and 30 feet wide, filled with cabinets containing 18,000 vacuum tubes interconnected by many kilometers of copper wire. This was the ENIAC (Figure 8.1), a 30-ton behemoth that was the world's first electronic computer. Now imagine that ENIAC had been given the task of solving a set of simultaneous linear equations that embodied 30,000 independent variables. With a team of people working around the clock to record intermediate solutions and feed them back into the computer (ENIAC had a limited amount of memory), ENIAC would still be chugging away more than 40 years later to solve the problem! A supercomputer using modern algorithms could solve the problem in an hour or so.

The speed and capability of the modern computer have tremendous implications for the practice of chemical engineering. In the future, computer programs incorporating artificial intelligence or expert systems will help engineers design improved chemical processes more efficiently. Complex computations based on fundamental engineering knowledge will allow engineers to design reactors that can virtually eliminate undesired by-products, making processes less complex and less polluting. New sensors, many of which will be miniature analytical laboratories tied to miniature electronics, will allow rapid and accurate measurements for control that are currently impossible. New chemical products that today are discovered predominantly through laboratory work – for instance, reinforced plastics that are as strong as steel and weigh less than aluminum or drugs with miraculous properties – may be discovered in the future by computer calculations based on models

that predict the detailed behavior of molecules.

Chemical engineers will lead this revolution. They will need to be trained to use advanced computer techniques for process design, process control, and management of process information. Advanced engineering development will be based more than ever on mathematical modeling and scientific computation. Reliable modeling at the microscale, the individual process unit scale, and the plant process scale will improve our ability to scale up processes in a few large steps, possibly bypassing the need for a pilot plant and saving the two or three years required to build and operate it. Process models capable of predicting dynamic behavior, operability, flexibility, and potential safety problems will permit these aspects of a process to be considered more fully earlier in the design stage. Because improved computers can perform the extensive computations required by such models, it will be possible to test alternative designs more quickly.

A chemical process must be designed to operate under a chosen set of conditions, each of which must be controlled within specified limits if the process is to operate reliably and yield a product of specified quality. Accurate, complex, computer-solvable models of chemical processes will incorporate features of the controls that are needed to maintain the desired process conditions. Such models will be able to predict the effects of process excursions and the control measures needed to correct them. Computer management of the process operation will rapidly initiate control correction of process excursions. The development of new types of process sensors will be essential to this degree of process control and will eliminate the time-consuming withdrawal of process stream samples for analysis.

The design of a commercial process can generate an almost uncountable number of possible solutions for seemingly simple problems. Even a decade's 10,000-fold increase in computational capability in terms of faster computer speeds and better algorithms does not permit a person to search among these alternatives, nor would such a search make strategic sense. Give engineers a design problem for which the best solution is obvious from today's technology, and they will quickly write down the correct solution without searching. If the solution is not obvious, they will often home in on the information needed and perform the computations that will expose the right solution quickly and with minimal effort. By using intuition and experience, they eliminate the need for testing every possible alternative. We need to understand how to use computer technology in much the same way, to solve complex problems where many of the decisions are based on qualitative information and insights that develop as the problem is attacked.

Encoding this activity in the computer involves a type of modeling in which the capabilities of the designer and his tools, the alternative procedures by which complex problem solving can be performed, and effective methods of information management are all incorporated. Advances in artificial intelligence, expert systems, and information management will revolutionize the automation of this activity, giving us computers that can display encyclopedic recall of relevant information and nearly human reasoning capabilities. A HAL 9000 of 2001: A Space Odyssey fame may indeed exist in the future.

Computer-generated visual information, for example, three-dimensional portrayal of proposed new designs, will be commonplace in the future. Communication will be in natural language, using both pictures and voice. This setting, which will address the need for new chemical processes and products by harnessing almost unimaginable computing power, will provide significant new research opportunities in chemical engineering.

Using The Computer's Potential

Each decade over the last 35 years has seen the processing speed of newly designed computers increase by a factor of about 100 owing to advances in the design of electronic microcircuits and other computer hardware. On top of this has been another 100-fold increase per decade in computer speed, thanks to more efficient methods of carrying out computations (algorithms). It is not widely appreciated that new algorithms have been as valuable as hardware design in improving computer performance. With the combination of improved computer hardware and better algorithms, effective computer speeds have more than doubled on average each year.

The availability of computing resources is also increasing rapidly. The actual and projected availability of high-speed supercomputers is shown in Table 8.1. The projection for 1990 – at least 700 computers of Cray I class – represents 35 times more available computing power than that available in 1980. While continued substantial investment in supercomputers is needed, support for better ways of using them should not be neglected. It is conceivable that a new algorithm could effectively increase the power of supercomputing for a specific problem by a factor of 35 overnight. During the last two decades, many developments in numerical analysis have had a profound impact on scientific computation.

Clearly computer technology has improved rapidly; there is little reason to doubt that it will continue to do so. The problem is now and will continue

PROCESS DESIGN IN THE TWENTY-FIRST CENTURY

It is April 2008. A process engineer for a medium-size chemical company is designing a process for a new series of products her company is developing. By talking to her computer and pointing to the screen, she indicates that the process needs a reactor and some separators, as well as recycle capability. The computer, using an artificial intelligence program tied to mathematical models, determines how the reactor temperature and pressure will influence the product yield and how the yield in turn will influence the amount of process stream recycle. The computer chooses the optimal types of separators and indicates how they should be sequenced for different process streams and products of the series. After 20 minutes on a teraflop machine (equivalent to 1 week of computing on a CRAY I of the 1980s), the computer indicates that the general process design is completed, having given partial information during the 20-minute computation.

The graphical output from the computer shows the process flowsheet, with several separation units and projected equipment and operating costs. It also flags information that is uncertain because it had to use thermodynamic data extrapolated from measured values. At the engineer's request, the computer shows several alternative flowsheets it had considered, indicates their projected costs, and tells why it eliminated each of them. Some of the flowsheets were eliminated because of high cost, others because they were considered unsafe, others because the startup procedures would be difficult, and still others because they were based on uncertain extrapolation of experimental data.

After perusal of these process options, the engineer asks the computer to select five designs for further study, and the computer produces a paper copy of the flowsheet and design parameters for each. She then tells the computer to prepare more rigorous designs from each of the five flowsheets. The computer questions the third design because it involves extensive extrapolation of known thermodynamic data. However, since the engineer feels that this may be one of the better designs, she asks the computer to notify the laboratory management computer, which is connected to a laboratory technician's terminal, to begin experimental determination of the missing thermodynamic data so that the design can be prepared. The computer reminds the engineer that precise control of process conditions will be essential for another of the designs and that a new sensor may be necessary. The engineer consults the artificial intelligence program, which tells her that either of two sensors being developed in another company department may fill her need. The engineer uses her computer to schedule a meeting with the manager of sensor development.

Two years later, the process is producing one of the new products. The time from design to operation was short enough that the company was able to capture a new market, and it plans to extend the business with related products of the series. The design engineer has developed a real-time dynamic simulation of the process and is running it on the company's parallel supercomputer to test strategies for producing the related products from the process equipment. She queries another computer to search the historical records of plant operation. She wants to know how well the dynamic model mirrors the actual plant operation and when the process parameters were last adjusted to give a better fit between the plant and the model. She feeds this information to her computer, which devises a comprehensive plan for scheduling production among four of the new products, with provision for revising the schedule as inventories and sale of the products change. A new business has been created.

to be the lack of people trained to apply computer technology to scientific and engineering tasks. The improvements suggested in Chapter 7 in terms of our ability to design and control better chemical products and processes will be made by chemical engineers who understand computers – not by computer scientists or by software engineers. The countries that understand this distinction will lead the world in chemical technology.

Year	Number of CRAY I – Class Supercomputers
1980	21
1085	142
1990	700-1,000

Table 8.1: Actual and Estimated Supercomputing Resources Available to Researchers in the United States, 1980-1990

Mathematical Models of Fundamental Phenomena

Chemical engineers have traditionally used mathematical models to characterize the physical and chemical interactions occurring in chemical processes. Many of these models either have been entirely empirical or have relied on crude approximations of the basic physics or chemistry of the process. This is because a typical chemical process comprises an assemblage of interacting flows,

transports, and chemical reactions. Accurate analysis and prediction of the behavior of such a complex system require detailed portrayal of the physics of transport and the chemistry of reactions, which calls for complex equations that do not yield to traditional mathematics. Nonlinear partial differential and integral equations in two and sometimes three spatial variables must be solved for regions with complicated shapes that often have at least some free boundary. The more accurate the model, the more mathematically complex it becomes, but it cannot be more complex than allowed for by the available methods for solving its equations.

Before the advent of modern computer-aided mathematics, most mathematical models of real chemical processes were so idealized that they had severely limited utility – being reduced to one dimension and a few variables, or linearized, or limited to simplified variability of parameters. The increased availability of supercomputers along with progress in computational mathematics and numerical functional analysis is revolutionizing the way in which chemical engineers approach the theory and engineering of chemical processes. The means are at hand to model process physics and chemistry from the molecular scale to the plant scale; to construct models that incorporate all relevant phenomena of a process; and to design, control, and optimize more on the basis of computed theoretical predictions and less on empiricism. Chemical engineers, using advanced computational methods and supercomputers, can now readily identify the important phenomena in a complex chemical process over the entire range of applicable conditions by exhaustive solution of detailed models. The benefits of investing in less empirical, more fundamental mathematical models are becoming clear:

- The capability to construct mathematical models that more fully incorporate the basic chemistry and physics of a system provides a mechanism for assessing understanding of fundamental phenomena in a system by comparing predictions made by the model with experimental data.
- Better models can replace laboratory or field tests that are difficult or costly to perform or identify crucial experiments that should be carried out. In either case, they will significantly enhance the scope and productivity of chemical engineering researchers in academia and industry.
- In process design, it is frequently discovered that many of the basic data needed to understand a process are lacking. Because most current mathematical models are not sufficiently accurate to permit direct scale-up of the process from laboratory data to full plant size, a pilot plant must be constructed. As models are improved, it may become possible to evaluate design decisions with more confidence, and bypass the pilot plant stage.

Process technologies for which the use of more comprehensive mathematical models can result in major improvements include those for biochemical reaction processing; high-performance polymers, plastics, composites, and ceramics; chemical reaction processing (e.g., reaction injection molding, reaction coating, chemical vapor deposition); microelectronic circuits; optical fibers and disks; magnetic memory systems; high-speed coating; photovoltaic and semiconductor materials; coal gasification; enhanced petroleum recovery; solution mining; and hazardous waste disposal. To date the most extensive use of supercomputer modeling has been in space age weapons technologies, where objectives, economics, and time frames differ from those in the chemical process industries. It is clearly in the national interest to stimulate the more extensive use of advanced computational methods and supercomputers in other industries critical to our worldwide competitive position. A program to encourage the greater dissemination of advanced computational techniques and hardware will offer challenges and opportunities to computational mathematicians and numerical analysts, to engineering scientists, to applications and software experts in firms that develop and manufacture supercomputers, and, above all, to perceptive leaders in high-technology process industries.

The following sections describe in more detail a number of areas in chemical engineering in which the ability to develop and apply detailed mathematical models should yield substantial rewards.

Hydrodynamic Systems

Much of the current computational modeling research in chemical engineering is concerned with the behavior of flowing fluids. The general system of equations that describe fluid mechanics, called the Navier-Stokes equations, has been known for more than 100 years, but for complex phenomena the equations are exceedingly difficult to solve. Only recently have methods been devised to treat such phenomena as shock waves and turbulence. Further difficulties arise when disparate temporal and spatial scales are present and when chemical reactions occur in the fluid. Solutions of the Navier-Stokes equations can be smooth and steady, or they can exhibit regular oscillations or even chaos. In some cases the fluid flow is enclosed by a rigid boundary with a complex shape, as in the extrusion of polymers; in others the flow is effectively unbounded and the solution must extend to infinity, as in atmospheric systems; and in still

Hypercubes

One thing that has not changed since the earliest days of the computer age is this: the fastest available computer is never fast enough to solve the most difficult problem of the day. Because of the limitations of current computers, simplifying assumptions about most physical systems must be made for the problem to be solved by available computer technology. For example, in petroleum reservoir simulation, available computer power dictates how many grid points can be used to describe the reservoir and how complex the thermodynamic model that describes the system can be. A computer capable of solving these complex systems without resorting to simplifying assumptions would have to be orders of magnitude faster than those available today.

Computer manufacturers have traditionally boosted performance by using faster components to build computers. But the overall architecture of computers has not changed since the 1940s, and the use of faster components is a strategy that is now running into diminishing returns. New computer architectures, based on parallel processing of sub-elements of the same problem, will be needed to achieve significant advances in speed to solve the complex problems of today and tomorrow.

One example of such a new approach is the hypercube architecture, in which many processors are linked together as a team to solve a single problem. A well-integrated team of cheap processing units can potentially out perform the most sophisticated single-processor machine. In addition, since each processor can have its own dedicated memory, the total system can have both more memory than current supercomputers and more memory in use at any given moment.

Standard programs must be broken into smaller pieces to run on a hypercube. Each processor is assigned the responsibility for calculations for a specific piece of a problem. For example, in petroleum reservoir simulation, each processor might be assigned a different section of the reservoir to model. In modeling a complex chemical plant, each processor might be assigned a different piece of equipment. As each processor proceeds, it informs the other processors of its results, so that all the other processors can incorporate the information into their respective portions of the overall calculation.

Hypercubes and other new computer architectures (e.g., systems based on simulations of neural networks) represent exciting new tools for chemical engineers. A wide variety of applications central to the concerns of chemical engineers (e.g., fluid dynamics and heat flow) have already been converted to run on these architectures. The new computer designs promise to move the field of chemical engineering substantially away from its dependence on simplified models toward computer simulations and calculations that more closely represent the incredible complexity of the real world.

others, such as the flow of blood in vessels, the boundary is deformable. Solution of the Navier-Stokes equations for systems of technological interest remains an exceedingly challenging task; supercomputers are needed to treat those systems that can be solved.

Polymer Processing

The development of polymers and polymer composites will benefit greatly from the availability of better computers and better algorithms. The inherent properties of a polymer are governed by the chemical structure of its molecules, but the properties of a finished polymer product are affected by the interactions among these molecules, which are strongly influenced by the way in which the material has been processed. While it is now possible to predict certain properties of polymers from their molecular structure, the ability to predict the effect of polymer processing steps on polymer properties is just being developed. Ideally it would be desirable to model all steps from the formation of the polymer through its processing and then predict the final properties of the material from structure-property relationships. Although such modeling is a formidable problem, it is becoming feasible with the advent of supercomputers and improved algorithms.

Petroleum Production

Computation is widely used in petroleum exploration and production by exploration geophysicists, petroleum engineers, and chemical engineers. As more sophisticated techniques are developed for locating and recovering petroleum, mathematical modeling is playing an ever-expanding role.

Once regions that may contain petroleum are located, local geological features must be sought that might have trapped the hydrocarbons. The discovery process is based on a kind of seismic prospecting in which geologic maps are constructed from reflected seismic signals generated by explosions or vibrations at the surface of the earth. These signals are reflected or refracted in varying degrees by different rock strata and are recorded by a set of receivers. Thus, the problem of interpreting signals can be likened to that of analyzing light beams reflected by an array of variously curved plates of glass of different reflectivities separated by liquids of different refractive indexes. The inverse mathematical problem of determining the earth structure and the properties of the strata from the recorded signals is extremely difficult (Figure 8.2).

After a hydrocarbon reservoir has been located, the flow of oil, water, gas, and possibly injected chemicals in the reservoir must be modeled. This challenge is particularly appropriate for chemical engineers working with petroleum engineers because of the important role played by molecular level interactions between oil, subsurface water, and rock. Models for fluid flow in porous media comprise coupled systems of nonlinear partial differential equations for conservation of mass and energy, equations of state, and other constraining relationships. These models are usually defined on irregular domains with complex boundary conditions. Their numerical solution, with attendant difficulties such as choice of discretization methods and grid orientation, is a challenging intellectual problem.

Once wells have been drilled into the formation, the local properties of the reservoir rocks and fluids can be determined. To construct a realistic model of the reservoir, its properties over its total extent – not just at the well sites – must be known. One way of estimating these properties is to match production histories at the wells with those predicted by the reservoir model. This is a classic ill-posed inverse problem that is very difficult to solve.

When or if the reservoir is successfully simulated, the engineer can turn to optimizing petroleum recovery, and theoretical ideas can be applied to models for various enhanced recovery methods to select optimal procedures and schedules (see Chapter 7).

Combustion Systems

Combustion is one of the oldest and most basic chemical processes (Figure 8.3). Its accurate mathematical modeling can help avoid explosions and catastrophic fires, promote more efficient fuel use, minimize pollutant formation, and design systems for the incineration of toxic materials (see Chapter 8). For example, modeling the initiation and propagation of fires, explosions, and detonations requires the ability to model combustion phenomena. Models of the internal combustion engine can shed light on the influence of combustion chamber shape or valve and spark plug placement on engine performance. Models at the molecular level can provide a fundamental understanding of how fuels are burned and how gaseous and particulate pollutants are formed. This can lead to ways to improve the design of combustion systems.

Mathematical models of combustion must incorporate intricate fluid mechanics coupled with the kinetics of many chemical reactions among a multitude of compounds and free radicals. They must also consider that those reactions are taking place in turbulent flows inside chambers with complex shapes. Because complete models of real combustors, incorporating accurate treatment of both fluid mechanics and chemistry, are still too large for present computers, the challenge is to construct simpler, yet still valid, models by using critical insight into the important chemical and physical phenomena found in combustors. Chemical engineers have the mix of expertise necessary to accomplish this.

Environmental Systems

The environment can be likened to a giant chemical reactor. Gases and particles are emitted into the atmosphere by industrial and other man-made processes, as well as by a variety of natural processes such as photosynthesis, vulcanism, wildfires, and decay processes. These gases and particles can undergo chemical reactions, and they or their reaction products can be transported by the wind, mixed by atmospheric turbulence, and absorbed by water droplets. Ultimately, they either remain in the atmosphere indefinitely or reach the earth's surface. For example, the hazes of polluted atmospheres consist of submicron aerosols of inorganic and organic compounds, which are formed by chemical reaction, homogeneous nucleation, or condensation of gases (Figure 8.4).

Models of atmospheric phenomena are similar to those of combustion and involve the coupling of exceedingly complex chemistry and physics with three-dimensional hydrodynamics. The distribution and transport of chemicals introduced into groundwater also involve a coupling of chemical reactions and transports through porous solid media. The development of groundwater models is critical to understanding the effects of land disposal of toxic waste (see Chapter 7).

Process Design

The primary goal of process design is to identify the optimal equipment units, the optimal connections between them, and the optimal conditions for operating them to deliver desired product yields at the lowest cost, using safe process paths, and with minimal adverse impact to the environment. Design is a complex problem that involves not only the quantitative computing depicted in the previous section, but also the effective handling of massive amounts of information and qualitative reasoning.

Computer-Assisted Design of New Processes

Designs for new processes proceed through at least three stages:

- Conceptual design – the generation (process synthesis) and their translation into an initial design. This stage includes preliminary cost estimates to assess the potential profitability of the process, as well as analyses of process safety and environmental considerations.
- Final design – a rigorous set of design calculations to specify all the significant details of a process.
- Detailed design – preparation of engineering drawings and equipment lists needed for construction.

The key step in the conceptual design of a new chemical manufacturing process is generating the process flowsheet (Figure 8.5). All other elements of computer-aided design (e.g., process simulation, design of control systems, and plant-wide integration of processes) come into play after the flowsheet has been established. In current practice, the pressure to enter the market quickly often allows for the exploration of only a few of the process alternatives that should be considered. To be fair to today's designers, it is possible to generate a very large number of alternative process paths at the conceptual stage of design, and yet experience indicates that less than one percent of the ideas for new designs become commercial. Thus, the challenge in computer-aided process synthesis is to develop systematic procedures for the generation and quick screening of many process alternatives. The goal is to simplify the synthesis/analysis activity in conceptual design and give the designer confidence that the initial universe of potential process paths contained all the pathways with reasonable chances for commercial success. The advances in computer-aided process synthesis that are possible over the next decade are dramatic. They include both an increasing level of sophistication (e.g., the synthesis of heat exchanger networks, sequences of separation processes, networks of reactors, and process control systems) and computational procedures that should make possible the identification of the most viable process option in a relatively short amount of time.

As the designer moves from conceptual design toward final design, he or she must analyze a number of alternatives for the final design. The development of large, computer-aided design programs (so-called process simulators) such as FLOWTRAN, PROCESS, DESIGN 2000, and ASPEN (or other equivalent programs used in various companies) has significantly automated the detailed computations needed to analyze these various process designs. The availability of process simulators has probably been the most important development in the design of petrochemical plants in the past 20 years, cutting design times drastically and resulting in better designed plants.

Although the available simulators have done much to achieve superior design of petrochemical processes, there is considerable room for improvement. For example, better models are needed for complex reactors and for solids processing operations such as crystallization, filtration, and drying. Thermodynamic models are needed for polar compounds. Moreover, the current process simulators are limited to steady-state operations and are capable of analyzing only isolated parts of a chemical plant at any given time. This compartmentalization is due to the limitations on computer memory that prevailed when these programs were first developed. This memory limitation resulted in a computational strategy that divided the plant into "boxes" and simulated static conditions within each box, iteratively merging the results to simulate the entire plant. With today's supercomputers, it is possible to simulate the dynamics of the entire chemical plant. This opens the way for dramatic advances in modeling and analysis of alternative process designs, because the chemical reactions that occur in manufacturing processes are usually nonlinear and interdependent, and random disturbances in the process can propagate quickly and threaten the operation of the entire plant. To nullify the effects of such disturbances, the designer must know the dynamics of the entire plant, so that control failure in any one unit does not radiate quickly to other units. It is now within our reach to integrate this sophisticated level of design and analysis on a plant-wide scale (including design and performance modeling of plant-wide control systems) into the computational tools used to analyze and optimize the performance of individual processes in the plant.

In the detailed design stage for a chemical manufacturing process, a chosen process design must be converted into a list of equipment items to be purchased and a set of blueprints to guide their assembly. The design is presented as a detailed process flow diagram (PFD), from which

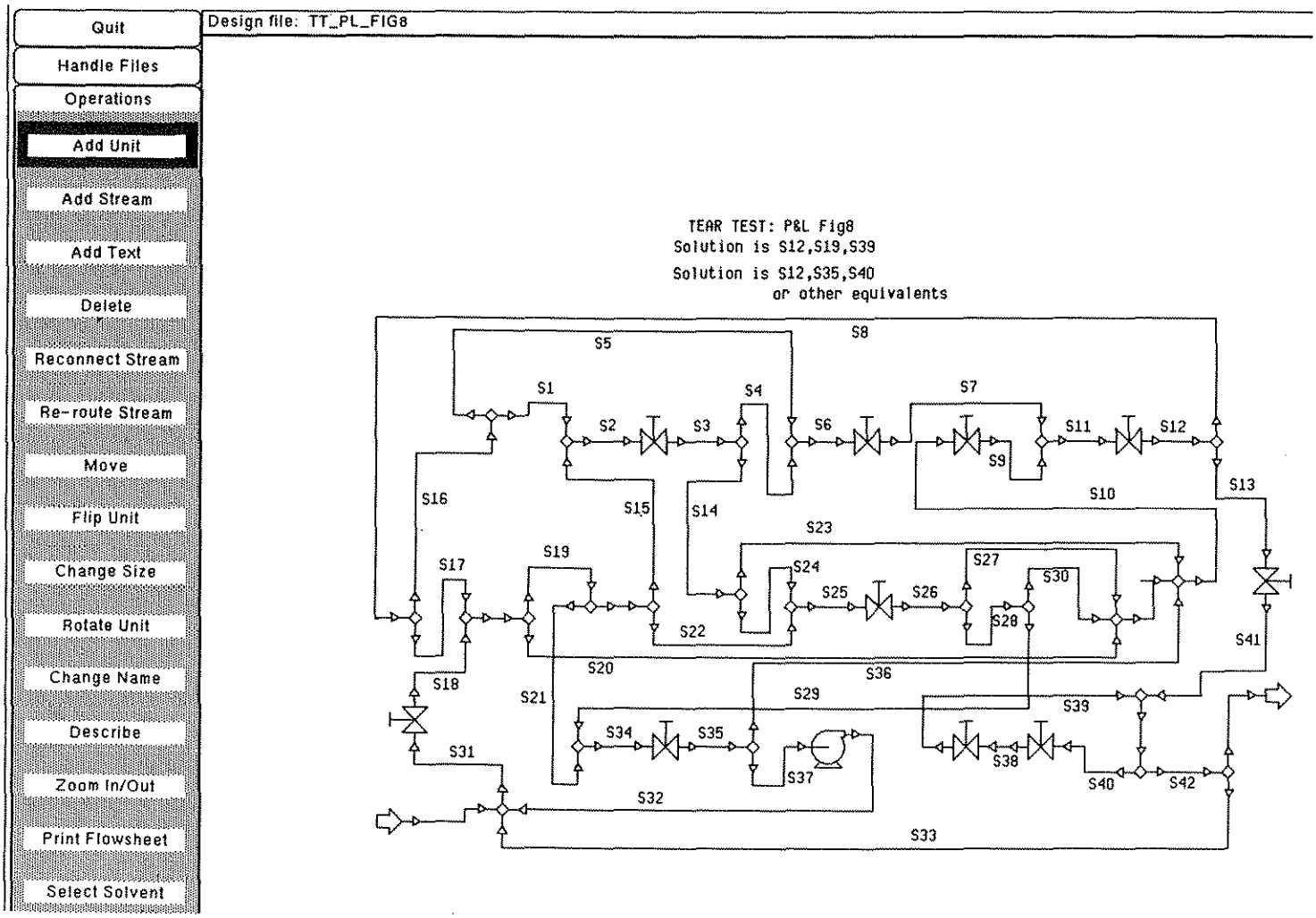

Figure 8.2: Example of a flowsheet generated by computer-aided process synthesis, as would be seen on the screen of a computer terminal. The column on the left side of the figure shows options available in the particular design program being run. Courtesy, Peter Piela, Carnegie-Mellon University

is constructed a list of all needed items of equipment, and piping and instrumentation diagrams (PIDs) that show the equipment and its interconnections. The next task is to establish the physical layout for the entire plant. Advanced computer-based drafting tools aid in all these activities.

Computer-Assisted Process Retrofitting

The preceding section focused largely on the design of new plants. However, these procedures can also be adapted to the retrofitting of existing plants. Retrofitting is generally undertaken to increase the capacity of a plant; to make use of a new technology such as an improved catalyst, a new material of construction, or a new unit operation; or to respond to a significant change in the cost of energy or raw materials. A fair amount of retrofitting in the chemical process industries in recent years has been undertaken to improve energy efficiency through plant-wide energy integration – retrofitting of about 50 processes to incorporate modern heat-exchanger network synthesis concepts has reduced energy requirements in the chemical industry by 30 to 50 percent. Retrofitting will continue to play a major role in the design of chemical plants as new procedures for computer-aided synthesis of separation systems are applied and research on process synthesis begins to yield large savings by helping existing petrochemical plants produce the same mix of products through more economical chemical reaction pathways.

We need to develop a systematic approach to analyzing the impact of making changes in the connections between process units or in the size of

units that are undertaken to improve operating costs, plant flexibility, or safety.

Research Opportunities in Process Design

The overall goal of process design research is to develop a systematic procedure, probably in the form of an interactive computer program, that contains design heuristics and interchangeable approximate and rigorous models that can lead an engineer from an initial concept to a final design as quickly as possible. The final design must include considerations of economics, controllability, safety, and environmental protection. We need to extend the conceptual and final design procedures that have been developed for petrochemical processes to processes for producing polymers, biochemicals, and electronic devices. We also must develop systematic synthesis/analysis procedures for studying batch processes analogous to the procedures that have been developed for studying continuous petrochemical processes.

There are some aspects of process design in which decisions are based primarily on past experience rather than on quantitative performance models. Problems of this type include the selection of construction materials, the selection of appropriate models for evaluating the physical properties of homogeneous and heterogeneous mixtures of components, and the selection of safety systems. Advances in expert systems technology and information management will have a profound impact on expressing the solutions to these problems.

In summary, systematic procedures must be developed for the following:

- generation of process alternatives;
- quick screening of process alternatives using both rule-of-thumb and short-cut calculations;
- inclusion of controllability, safety, and environmental factors in the initial design;
- more detailed screening of a small number of promising design alternatives;
- design of the process and management of its construction;
- use and extension of expert systems concepts to handle aspects of design that deal with a mixture of qualitative and quantitative information; and
- retrofitting of existing plants.

Process Operations and Control

Process operations and control have a tremendous impact on the profitability of a manufacturing operation. In some cases, they can determine the economic viability of a manufacturing facility. For example, DuPont's Process Control Technology Panel has estimated that if DuPont were to extend the degree of computer process control that has been achieved at a few of its plants across the entire corporation, it would save as much as half a billion dollars a year in manufacturing costs. If DuPont's numbers are representative, the entire chemical industry could save billions of dollars each year through more widespread application of the best available process control. This could be the single most effective step that the U.S. chemical process industry could take to improve its global competitive position in manufacturing.

Why are such savings suddenly possible? Because of the explosive developments in computer technology, research on operations and control is no longer constrained by lack of computing power. In particular, the traditional boundaries between design, control, optimization, simulation, and operation are disappearing. Control is becoming a part of process design; simulation and optimization are becoming components of control design.

Research opportunities in process operations and control lie in three areas:

- collection of information through process measurements;
- interpretation and communication of information by use of process models; and
- utilization of information through control algorithms and control strategies for both normal and abnormal operation.

Measurements

The essence of process control is to take appropriate and quick corrective action based on measured information about the behavior of the process. The concept of the process is contained in a process model, and measurements are used to evaluate the degree to which the process conditions deviate from those of the model. When a mismatch occurs between actual process conditions and those postulated by the model, a control and operating strategy is invoked to correct the process conditions. A critical interrelationship exists between measurements and operating/control strategy, one that is too often neglected. The control strategy depends on what information is or can be available, even while it dictates which measurements are needed. This is perhaps best illustrated in a number of manufacturing processes in cutting-edge technologies, where control and operating strategy is circumscribed by the lack of appropriate sensors for many critical process variables. Conventional estimation techniques are used that infer the values of unmeasured variables from measured variables, but these provide imperfect guidance for process control.

Even something as empirical as process measurement cannot be divorced from the need for good process modeling. In the absence of a good model, it may not be known what variables affect process operation or product quality and should therefore be measured or estimated.

Process measurements are subject to errors. Random (stochastic) disturbances are ubiquitous, and gross or systematic errors can be caused by malfunctioning sensors or instruments. The detection and elimination of these errors are essential if the data are to be used for process operations and control. The success of this screening depends on the measurements themselves, the failure data available, and the process control strategy. At the present time, diagnostic programs are not applied to most sensor failure data. The detection and remediation of significant errors in measurements for process control pose interesting research opportunities.

Interpretation of Process Information

The quality of an operation and control strategy depends on the quality of the model on which it is based (Figure 8.6). We are only beginning to understand this relationship quantitatively, even in the relatively simple context of the feedback control of linear systems. Even if it is assumed that the structure of the process model is correct, we do not yet know how to translate uncertainties in model parameters into uncertainty in the performance of the control system. A more difficult problem is to assess the effect of an incorrect model structure, such as a wrong set of basic equations, on the performance of the control strategy on which it is based. Understanding the effect of model-process mismatch on control system performance provides a critical research opportunity.

In the context of operations and control, simulations can be used to test new process strategies as well as to train operating personnel to control the process and to respond to emergencies. The increasing use of simulation in process control requires that the cost of dynamic simulation be brought down. This could be done by taking advantage of new developments in computers, such as new user interfaces, computer architectures, and languages, and by developing faster numerical integration algorithms for ordinary differential equations.

Alarm management also requires research. Modern chemical plants usually have audible and visual annunciators to warn operators when key variables deviate from acceptable or safe values. A process upset in a plant that has several interconnected units with many feedback controls can set off multiple alarms, and the consequences of misinterpreting the alarms can range from inefficient process operation to outright disaster. When the alarm sounds, the operator must decide quickly what action to take. A hybridization of expert systems and process control systems can assist the operator in interpreting process status after an abnormal event. The need for better handling of abnormal events makes research in artificial intelligence of great importance to the chemical industry.

Integration of Process Design with Control

Most continuous plants are now designed for steady-state operation with little regard for the ease (or difficulty) with which the steady state can be maintained through control. Such a plant can be difficult to control once it deviates from the steady state.

Design and control have traditionally been treated separately for the following reasons:

- The problems in each area alone are exceedingly complex.
- The interactions between design, control, and optimization are poorly understood.
- The computational requirements of an integrated approach to design and control have been beyond the capability of available hardware and software.

For example, a chemical plant might be designed to achieve high efficiency by integrating the operation of many individual process units across the plant (e.g., by using waste heat from one unit as an energy source in another unit). However, the tight coupling of process units generally makes the entire plant more difficult to control. Therefore, this is a factor that must be considered at the design stage. No methodology currently exists for including this consideration in plant design; its development constitutes a significant research opportunity.

The supercomputer power that is becoming available will provide the opportunity to combine process and control system design – including optimization – into one large problem that can be solved in a way that accounts for their interactions. The success of such a consolidation will depend on the development of approximate compatible models and of techniques to relate model quality to performance.

Robust and Adaptive Control

Control systems are designed from mathematical models that are generally imperfect descriptions of the real process. It is essential that control systems operate satisfactorily over a wide range of process conditions.

A Revolution In Process Control

Until recently, the chemical process industries have largely tried to solve difficult control problems by using simulation, case studies, and ad hoc on-line adjustment of controller knobs – a procedure that can require personal intuition and continuous human supervision of the controls. These industries did not use modern control techniques because available control theory did not address practical issues. The control theory that was dominant in the 1960s and 1970s assumed that the designer had a linear mathematical model of the process to be controlled as well as a substantial body of fixed knowledge on likely disturbances and the inherent "noise" in the measurements made by process sensors. Such a linear process control theory is built on fatal shortcomings: there are no truly linear processes and there are no fixed, known spectra of information on disturbances and measurement noise. Controllers designed on the basis of linear process theory will fail in the real world of nonlinearity and uncertainty.

New research advances in control theory that are bringing it closer to practical problems are promising dramatic new developments and attracting widespread industrial interest. One of these advances is the development of "robust" systems. A robust control system is a stable, closed-loop system that can operate successfully even if the model on which it is based does not adequately describe the plant. A second advance is the use of powerful semi-empirical formalisms in control problems, particularly where the range of possible process variables is constrained.

The development of "internal model control," a design technique that bridges traditional and robust techniques for designing control systems, has provided the framework for unifying and extending these advances. It is now available in commercially available design software.

The combination of these advances is revolutionizing process control, spawning unprecedented research activity in both academia and industry.

Thus, the control algorithm must provide for control of the process even when the dynamic behavior of the process differs significantly from that predicted by the model. A control system with this characteristic is sometimes called robust. In fact, a traditional disregard for the model error problem is one of the main reasons for the frequently cited gap between theory and practice in process control. Industry needs algorithms that are robust rather than ones that "get that last half percent performance." Control strategies that work all the time within reasonable limits are better than those that work optimally some of the time but that frequently require reversion to manual control.

Because a process often changes over time, its model parameters must be continually updated; in extreme cases, the basic model must be reformulated. An adaptive system is a control system that automatically adjusts its controller settings or even its structure to accommodate changes in the process or its environment. The problem of model-plant mismatch is of crucial importance in the design of adaptive controllers for processes since it is that very mismatch that drives changes in the controller parameters. The engineering theory and methodology for designing reliable adaptive controllers for chemical processes are in the earliest stages of development.

Finally, there are always process operations in which neither classical nor modern control is effective. Such operations may require qualitative decision making or the use of past knowledge. Artificial intelligence techniques offer promise for control system design in these cases.

Batch Process Engineering

The production of fine and specialty chemicals, which are usually made by batch processes, is becoming increasingly important and competitive (Figure 8.7). The efficient operation of multiproduct and multipurpose batch plants offers a variety of challenging research problems for chemical engineers. Most industrial batch chemical operations are now scheduled by intuitive, ad hoc methods that consist of modest variations around historical operating patterns and that make little or no use of computer technology. It is now widely recognized that the scheduling problems associated with batch processes are immensely complex and, in fact, are among the most difficult combinatorial problems known. Limited progress has been made in using mathematical models in the simplest types of batch process scheduling. Current algorithms are too computationally demanding and complex for industrial use. An important intellectual challenge is to generate a unified field of batch process engineering theory and to put it into a practical context by using case studies.

Linear control theory will be of limited use for operational transitions from one batch regime to the next and for

the control of batch plants. Too many of the processes are unstable and exhibit nonlinear behavior, such as multiple steady states or limit cycles. Such problems often arise in the batch production of polymers. The feasibility of precisely controlling many batch processes will depend on the development of an appropriate nonlinear control theory with a high level of robustness.

While startup and shutdown occur relatively infrequently in large continuous plants, they are inherent in batch plant operation. Most startup and shutdown procedures, whether devised empirically or theoretically, are designed to follow a recipe of actions with no feedback. Thus, if upsets occur, there is often no way to change the startup or shutdown in time to avoid unwanted process excursions. Procedures are needed that incorporate feedback and adaptive techniques to the problem of plant startup and shutdown.

Process Sensors

If we had a completely accurate model of a process and accurate measurements of process disturbances at their inception, then corrective action could be taken directly without the need to measure the output streams from the process after the disturbance has propagated through it. But because we generally do not have adequate models, the output streams of processes must be measured for the purpose of feedback control.

The sensor is the "fingertip" of the process control system. The principal challenge in process sensing is the development of analytical sensors, particularly for determining process stream composition. Such sensors eliminate the need to withdraw samples to determine process and product parameters, a practice that should be minimized because of inherent problems (e.g., samples of reactive intermediates may be toxic or otherwise dangerous, or the intervention represented by withdrawing a sample may affect process operation). Since it is important for process control not to disturb the normal operation of the process, sensors are needed that can operate in the environment of the process stream. The key to meeting this challenge is a fundamental understanding of the physical and chemical interactions at the sensor-environment interface and, in particular, the transport and kinetic processes that occur there.

Future Sensor Developments

The techniques used in the chemical processing of electronic microcircuits (see Chapter 5) are being adapted to the microfabrication of two- and three-dimensional structures for solid-state sensors. These techniques will permit the integration of transducers, optoelectronics, signal-conditioning and data-processing devices, and micromechanical devices into extremely small packages. Reduced size offers advantages in thermal uniformity and response speed; shock and acceleration resistance; and reduced weight, volume, power, and cost.

Solid-state sensors may be developed that will be responsive to a broad range of acoustic inputs, electromagnetic radiation, ionizing radiation, and electrochemical stimuli. Response elements may be tailored for high selectivity among ions, free radicals, or specific compounds. Alternatively, elements with low selectivity are also useful because information from an array of such sensors, each with a different but known broad response, can be processed to provide quantitative analysis of a complex mixture. Complex mixtures also lend themselves to chromatographic analysis. It has been shown that gas chromatographic data can be analyzed on a silicon chip, although with some loss in recognition reliability. Combinations of gas or liquid chromatography or capillary electrophoresis of microsamples with mass spectrometry may be developed to provide superior performance.

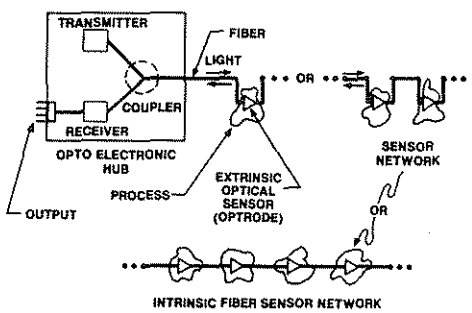

Figure 8.4: Configurations for several different kinds of optical fiber sensing systems are shown. The common factor in all these systems is the use of an optical fiber as an integral element in the system, either to carry light to and from discrete sensors (often referred to as optrodes), or as sensitive elements themselves (intrinsic fiber sensors). Courtesy, AT&T Bell Laboratories.

The development of biological sensors is taking place at a rapid pace. Biological sensors analyze chemical mixtures using biological reagents of exquisite specificity – for example, enzymes, immunoproteins, monoclonal antibodies, and recombinant nucleic acids. Such sensors may permit the analysis of fast reactions of species in very dilute media. Multicomponent biological sensors may be able to perform complex analyses that involve multiple reactions, with automatic regeneration of the biochemical reagents or removal of interfering species.

Unfortunately, current biological sensors are extremely delicate. Even when the biological reagents are immobilized on a solid carrier, such sensors require careful construction and frequent recalibration, are not always amenable to automation or unattended operation, and sometimes

have inconsistent dynamic response and limited life. Although biological reagents are ideally suited for some applications, particularly those in relatively mild environments, they may not survive the harsher conditions often found in process industries. Here again, miniaturization of the biological sensor and its direct integration into an optoelectronic transducer, potentiometric electrode, or membrane are promising approaches. With the current worldwide interest in biotechnology, major innovations in biological sensors can be anticipated.

Further advances in optoelectronics will allow the development of instrumentation with no electrical components in the sensor. These devices will operate by transmitting probe light from a remote source to the process sensor with an optical fiber light guide. In the sensor, the light signal will be altered by the sensed environment (e.g., by absorption of certain wavelengths, fluorescence, or scattering) and will thus be "encoded" with information. The encoded signal is transmitted through the optical fiber to a transducer that produces an electronic signal. The advantages of such systems include inherent safety, low signal attenuation, and the ability to multiplex signals in the optical fiber. Such instrumentation can incorporate additional chemical, biological, and electronic components and is likely to play a major role in many future sensor systems.

Future sensors and their associated data processing elements will need capabilities beyond those required for the simple measurement of process variables, such as periodic self-calibration against known standards, automatic compensation for environmental or other interferences, signal conditioning including linearization or other variable calculation, and fault recognition and diagnosis. Some of these capabilities are now available to a limited extent. Others will become available with the continued development of integrated sensors and data processing instrumentation. Arrays of sensors have already been mentioned in connection with complex mixture analysis, but they may also be used to provide redundancy, fault detection, and data reconciliation.

Research Opportunities

The availability of high-quality, real-time information on the conditions and composition of the process stream will permit engineers to develop a completely new generation of process control strategies. The physical, chemical, and biological phenomena at the sensor/process interface must be understood and translated into sensor technology. Chemical engineers are well positioned to contribute to the development of improved process sensors in a variety of ways, including

- Work in interdisciplinary collaborations with electronic engineers, biologists, analytical chemists, and others to elucidate the biological, chemical, and physical interactions to be measured;
- Application of fundamental principles of reaction engineering and transport phenomena to the design of sensor surfaces;
- Development of new process control systems and operation strategies in response to improved capabilities for measurement; and
- Determination of the implications for process design of wholly new types of process sensors.

Process Engineering Information Management

In the next decade, competition among industrialized countries will be influenced by the way in which information and knowledge are managed in industry. The challenge is to be the first to find relevant information, to recognize the key elements of that information, and to apply those elements in the manufacture of desired products.

Computer technology will continue to provide new generations of hardware and software for fast information processing and low-cost storage and retrieval. The use of computers for information management and decision making will be essential, and advanced capabilities in user interfaces and networking will bring new dimensions to this application. For example, current on-line literature search systems allow data sharing among many users, significantly increasing individual productivity. However, this technology is generally only used to manage well-organized data; basic research is needed to apply it to engineering data, which are not as well organized.

A process engineer will need to be able to store and access relevant data rapidly in order to carry out process development and design in less time and to solve problems arising from new and complex design requirements (e.g., designing for multiple objectives of profitability, safety, reliability, and controllability). To provide for rapid data storage, access, and transfer, new generations of computer hardware (bulk storage, network, and work stations) and software (data bases) will be needed. Some specific research challenges for chemical engineers, working together with computer scientists and information specialists, follow.

- Most chemical manufacturing processes in the future will be monitored and controlled by computer. Process data will be collected continuously and stored either locally or in a central data base. Research is needed to develop mutually compatible, efficient algorithms for storing and retrieving process data. In addition, computerized procedures

will be needed for sifting through voluminous process data for information to use in process improvement and in the generation of new processes.

- Methods must be developed for storing judgments, assumptions, and logical information used in the design and development of processes and models.
- Procedures and methods will be needed for retrieving and operating on other types of imprecise data.
- Efficient transfer of information among engineers and designers will depend on how easily these data can be accessed. The special needs of chemical engineers in this area – the particular ways in which they generate, manage, and use information – merit study.

Implications of Research Frontiers

The speed and capability of the modern computer, as well as the developing sophistication of chemical engineering design and process control tools, have tremendous implications for the practice of chemical engineering. Chemical engineers of the future will conceptualize and solve problems in entirely new ways. There are two bottlenecks to the application of these powerful resources, though. First, there are not enough active research groups at the frontiers of computer-assisted process design and control. A larger effort is needed in order for the field to keep pace with the expanding power of available computers. Second, many chemical engineering departments lack the computational resources needed to fully integrate advances in design and control into their curricula. For the full potential of the computer to be realized in improved design of chemical products and the improved design and operation of processes to produce them, chemical engineers must be broadly versed in advanced computer technology. This can only happen if they have access to state-of-the-art computational tools throughout their educational careers, not in an isolated course or two.

Making this broad access and utilization of the computer in education possible will require substantial government, academic, and industrial funding to provide both hardware and software. In some cases, groups may need remote access to networks of supercomputers. In other cases, dedicated array processors and other computational hardware may be required in the chemical engineering department. If this country is to maintain a leadership role in chemical technology, critical needs for both research support and facilities acquisition must be addressed. The status of funding in this field and a specific initiative to achieve the goals outlined above are discussed in Chapter 10 and Appendix A.

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Thanks from Washington

by Henry McGee, Washington DC
AIChE Meeting Program Chairman

With many fine sessions from the CAST Division, the Washington DC meeting was a great success. Meeting attendance was among the top two or three in all of AIChE history. The meeting had a number of innovations in both technical content and in organization. Although most of this technical content came from the established groups and Divisions in the usual way, some special speakers and sessions either originated from the Meeting Program Chairman and his Committee, or else were midwifed by the MPC. One of these latter types of sessions was on Global Climate Change. Interestingly, this session was broadcast live by the Voice of America. This particular example of public attention was unique at our Washington affair and is certainly not common in AIChE history.

The Supersessions were conceived as teaching exercises wherein new and exciting avenues for the potential exercise of chemical engineering expertise might be presented to us. The speakers were, in general, not baptized chemical engineers, and the format for their presentations was meant to be attractive and compelling. The Biotech Supersession was certainly one of the most compelling and best attended of these; it attracted an audience of perhaps 700 to 800 people. In this session, we learned what chemical engineers might do with unusual marine organisms collected from Australia's Great Barrier Reef. And we learned that recombinant DNA has a proper place in chemical engineering departments. All of this is definitely not dull. Perhaps CAST will want to state such a Supersession at a forthcoming meeting. I hope so. In any event, thanks again for your sessions, which contributed so much to the success of the Washington DC meeting.

The AIChE Management Division

by M. Tayyabkhan, Chairman, Management Division

Greetings to the members of CAST Division. I welcome this opportunity to tell you a little bit about the bold plans and valiant attempts in the Management Division that we hope will turn into an exciting program for members of our division. It is a special privilege to talk to you, since, I have been a member of the CAST division ever since it was formed.

The Management Division is younger and smaller than CAST; it was formed in 1975 and has about 800 members. Our members are predominantly affiliated with industry. Jim Mathis recently carried out a very interesting survey and produced a very clear picture of the profile and the interests of our members. If any of you would be interested in such information, please contact me at (609) 924-9174.

As a Division, we are concerned with three levels of management, which are:

(1) Top management
(2) Middle management
(3) Professionals, including recently promoted first-level supervisors, who aspire to be in management

We have members from each of these levels. We also have contacts with individuals in each of these levels who are not members of AIChE.

Top management and our contacts with them are, by and large, resources for us and for AIChE. Periodically our Division organizes, in close cooperation with the Executive Director of AIChE, special one-day meetings where the top management from industry discusses with the Executive committee of AIChE issues of interest to chemical engineering professionals. In the recent past these discussions have included subjects such as supply and demand of chemical engineers, impact of corporate take-overs, opportunities for chemical engineers in non-conventional industries, and so forth. In this context we are always looking for persons with ideas and contacts. If you have any, please come forward.

Middle management from industry does not take as much interest in the institute as we would like them to. Many of them may have felt that their needs were not met by the activities of AIChE and have directed their attention elsewhere. We believe that we need to develop mechanisms that would get them involved with us.

To this end, we plan to help local sections of AIChE organize special lunches, say two times a year, for middle management in the chemical process industry in several cities of the country. We hope to assign a member of the Division to be a helper to the local section in that city. The lunches would be attended by the invited persons in middle management, officers of the local section, and several members from the Management Division who live in the city. These lunches would offer individuals in the middle management of one company an opportunity to meet individuals from other companies in similar positions. This may prove to be an enticement for middle managers to attend.

In an attempt to meet the needs of the newly appointed managers and aspiring managers, we are encouraging members of our Division to make presentations on management skills at local sections. We plan to provide a few speakers with interesting talks on management subjects to the Speakers Bureau that is run by AIChE. At the same time, we hope to develop programs at national meetings that deal with first-level management skills and with organizational and behavioral matters.

Let me now turn my attention to our programming activities. The CAST Division is extremely strong in this area, and we can learn from you. Most of our programming committees would benefit from joint programming with other divisions, because there is natural overlap in some areas of interest. I invite the CAST Division to consider joint programming with us. For your information, I am listing our programming committees and their chairmen. Please feel free to contact them if you have suggestions.

Chairman of area 5 (Management Div): Al Wechsler (617) 864-5770

5(a) Management of Research
Chmn: Tom Hanley
(904) 487-6144

5(b) Project Management
Chmn: Hebab Quazi
(818) 300-6898

5(c) Management Sciences:
Irene Farkas-Conn
(312) 842-6388

5(d) Plant and Manufacturing Management:
Bob Gilbert
(713) 474-8500

5(e) Corporate Management
Chmn: Jim Mathis
(201) 522-8764

5(f) Environmental and Legal
no chairman

5(g) Personnel Management:
Marvin Livingood
(502) 459-8888

5(i) Private Practice and Consulting
Chmn: John Grant

5(j) Technology Transfer
Chmn: Mike Tayyabkhan
(609) 924-9174

5(k) Project Analysis and Economics:
Jim Weaver
(813) 378-1287

Several of us in the Management Division, specially on the board and the executive committee, are quite active in use of computing and electronic mail. In this area, I believe, our divisions have an opportunity to work with each other. One of the challenges we face is that the academic members of AIChE have access to and use BITNET, whereas the industrial members use one of two or three popular commercial systems. We must have good communications between our industrial and academic members and bridge the gap between the different e-mail systems in an efficient and cost effective manner. Peter Rony and I are planning to experiment with solutions to this problem and we welcome suggestions and other participants.

In closing, I want to thank you and your forever experimenting editor for letting me address you. Please contact me with your suggestions and questions (Telephone (609) 924-9174; Telex 4933567 MTTUI; MCImail ID 348-9468; USmail 62 Erdman Ave., Princeton NJ 08540), or better still, join our Division and show up at our meetings and sessions.

A Commitment to the Betterment of the Process Industries

by Vincent S. Verneuil, Jr.

Simulation Sciences Inc. is proud to sponsor the Computing in Chemical Engineering Award given annually by the Computing and Systems Technology Division. Sponsorship of this award, which gives recognition for outstanding contribution in the applications of computer and systems technology, is one important way that SimSci® lives up to its Mission Statement commitment to ". . . contribute to the overall betterment and productivity of the process industries."

Last year's recipient, Professor James M. Douglas, exemplifies how one individual can make an outstanding contribution to our industry through creative, innovative thinking. His systems approach to process design provides us with new insight and methodology for creating and evaluating process alternatives. We hope that the recognition given Professor Douglas will not only encourage him to continue his work, but will inspire the rest of us to try harder to make our industry a little better.

We are indeed fortunate to participate in the dynamic changes taking place in our industry at this time. With the advent of faster and more economical computers, distributed processing, and new methods, data and expert systems for designing and optimizing process plant performance, our ability to develop more powerful, yet easier to use, computer software and put it in the hands of the practicing engineer has never been greater.

Over the years, SimSci's commitment to the betterment of the process industries has included grants to selected universities for research, and the free use of our PROCESS® simulator. Today, approximately 200 universities worldwide use PROCESS as a teaching tool in their undergraduate design courses. We believe that student exposure to commercial simulation tools within the context of their thermo, design and optimization courses is excellent preparation for their industry careers.

During SimSci's 22-year history, we have continuously developed and expanded our simulation capability in response to advances in technology and the needs of our customers. Each year we have added new capabilities and released new, improved versions of our programs. And, as needs change, we have developed entirely new generations of our programs to keep current with new technologies.

With the introduction this year of PRO/II®, our fourth generation simulator, the convenience, accessibility and ease of use of our simulator has been greatly increased. PRO/II input/output graphics and flowsheet plots, along with case compare features, aid productivity and flowsheet understanding. Built on a new structure, database and graphics environment, it is designed to operate efficiently in today's computing environment, and to provide a platform for an integrated process engineering system.

Simulation Sciences Inc. is proud to be a part of the process industries and to make our small contribution to the advancement of computerized process engineering. There are many outstanding contributions made to our industry daily that go with little or no recognition outside of a small local audience. We are happy to sponsor one award, and hope that it helps all of us renew our commitment to the betterment of our industry.

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Meetings and Conferences

The following items summarize information in the hands of the Editor by January 26, 1989. From this point forward, the deadlines for the two issues of CAST Communications – called the Winter and Summer issues – will be approximately several weeks after the Fall and Spring AIChE meetings, respectively. These revised deadlines will give CAST division members who are active in CAST programming activities sufficient time after AIChE meetings to send last-minute information to both the Publications Board Chairman (Jeff Siirola) and the Editor of the newsletter (Peter Rony). We prefer that all communications with us be

done in electronic form, either with MS DOS formatted diskettes or else with messages sent electronically over BITNET. The most up-to-date listing of proposed sessions and Calls for Papers will be maintained electronically by the Publications Board Chairman.

To repeat comments made in the "About This Issue" editorial: "This issue will be one of three to be published this year: Volume 12, No. 1, the Fall 1988 issue, delayed to accommodate the Calls for Papers for the 1989 San Francisco AIChE meeting; Volume 12, No. 2, also known as the "Winter 1989" issue, a short issue containing Part 2 of the Frontiers in Chemical Engineering: Research Needs and Opportunities article, meeting announcements, and Calls for Papers, and delayed several months from the normal publication schedule for the "Winter" issue; and Volume 12, No. 3, also known as the "Summer 1989" issue, which will be published on time in August 1989 and will contain the Award Address (including copies of his illustrations) by Professor J. D. Seader, "Computers and Chemical Engineering Education," at the CAST Division banquet at the Washington D.C. AIChE meeting. This revised schedule has been developed with the cooperation of both the Publications and the Programming Board chairmen. By the end of the summer, we hope to have all of the CAST programming area chairmen linked electronically by BITNET. A listing of tentative programs, first calls, final calls, and a program schedule for the next meeting will be updated every several months and made available to all CAST Division members (who have access to BITNET) on the LSUCHE GRAND file server at the Department of Chemical Engineering, Louisiana State University. We are still hoping that AIChE headquarters in New York will be able to gain access to a local BITNET node.

Please send CAST Division session information, Calls for Papers, meeting, and short course announcements to me immediately by February 1, 1989 for inclusion in the "Winter 1989" issue of CAST Communications.

Peter R. Rony,
Editor, CAST Communications

Houston AIChE Meeting
(April 2-6, 1989)

The programming booklet for the 1989 Spring National Meeting and Petrochemical Expo '89 at the George R. Brown Convention Center in Houston, Texas has already been received by all CAST Division members.

Area 10a Sessions

1. **Applications of Expert Systems in Process Engineering.** Babu Joseph (Chairman), Department of Chemical Engineering, Washington University, St. Louis, MO 63130, (314)889-6076 and Heinz A. Preisig (Vice Chairman), Department of Chemical Engineering, Texas AM University, College Station, TX 77843-3122, (409)845-0386.

2. **Computer-Aided Process Modeling and Simulation,** Lorenz T. Biegler (Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412)268-2232 and Ralph W. Pike (Vice Chairman), Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803, (504)388-6910.

3. **Bioprocess Design and Simulation: Issues and Tools.** Michael M. Domach (Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412)268-2246 and Randy Field (Vice Chairman), Aspen Technology, Inc., 251 Vassar Street, Cambridge, MA 02139, (617)497-9010.

4-5. **Retrofit Design Technique and Applications I and II.** Rajeev Gautam (Co-Chairman), Union Carbide Corporation, P.O. Box 8361, South Charleston, WV 25303, (304)747-3710 and H. Dennis Spriggs (Co-Chairman), Linnhoff March Inc., P.O. Box 2306, Leesburg, VA 22075, (703)777-1118.

For further details concerning Area 10a sessions and scheduling, please contact Michael F. Doherty (Area 10a Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413)545-2359.

Area 10b Sessions

1. **Expert Systems in Process Control**

2. **Control of Separation Operations**

Area 10c Sessions

1. **Innovative Uses of Spreadsheets in Engineering Calculations I and II.** Kris Kaushik (Co-Chairman), Shell Oil Company, P.O.Box 2099, Houston, TX 77252-2099, (713) 241-2098 and Keshava Halemane (Co-Chairman), University of Maryland, Department of Chemical Engineering, College Park, MD 20742, (301) 454-5098.

2. **Plant-Wide Use of Computers in Process Operations.** Ed Rosen (Co-Chairman), Monsanto Co. F2WK, 800 N. Lindbergh, St. Louis, MO 63167, (314) 694-6412 and Irven Rinard (Co-Chairman), City College of New York, 138th St. and Convert Ave., New York, NY 10031, (212) 690-4135.

3. **Personal Computers in Planning and Scheduling.** Mike Tayyabkhan (Co-Chairman), Tayyabkhan Consultants, 62 Erdman Avenue, Princeton, NY, 08540 and Ed Bodington (Co-Chairman), Chesapeake Decision Science, P.O. Box 275, San Anselmo, CA 94960.

4. **On-Line Fault Administration.** Mark Kramer (Co-Chairman), Dept. of Chemical Eng., Room 66-542, Massachusetts Inst. of Tech., Cambridge, MA 02139, (617) 253-6508 and V. Venkatsubramanian (Co-Chairman), Chem. Eng. & Applied Chemistry, Columbia University, New York, NY 20027, (212) 280-2561.

For further details concerning Area 10c sessions and scheduling, please contact Ignacio Grossmann, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268-2228.

European Symposium on Computer Applications in Chemical Industry, Erlangen, Federal Republic of Germany
(April 23–26, 1989)

The conference topic will be subdivided into four subject groups:

- Expert Systems and Data Bank Management Systems
- Computer Integrated Production
- Process Synthesis and Design
- New Developments in Computing

The symposium subjects will be treated in plenary papers, oral (about 40), and poster contributions, plus a roundtable discussion. About 30 minutes, including discussion, will be available for every oral contribution, while the time foreseen for the display of posters will be one day. The final decision on oral or poster presentations will reside with the Scientific Symposium Committee.

All manuscripts will be printed and published in one volume and be available for distribution to all symposium participants at the beginning of the meeting. A number of facilities will be available at the symposium for the demonstration of programs and data banks. Interested persons are invited to inform the organizers about their participation by October 1988. Further details will be worked out on the basis of requests received and will be communicated at the beginning of 1989. The symposium language will be English.

The symposium is organized by DECHEMA Deutsche Gesellschaft fur Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V., Frankfurt am Main in collaboration with members of the Dechema-Fachausschuss Anwendung elektronischer Rechengerate in der Chemischen Technik, and members on the Working Part on use of Computers in Chemical Engineering of the European Federation of Chemical Engineering.

Correspondence and Secretariat: DECHEMA, Attention Mrs. L. Schubel, P. O. Box 97 01 46, D-6000 Frankfurt am Main 97, West Germany. Phone (069) 75 64-235/209.

Short Course

Advanced Process Control, McMaster University
(May 15-19, 1989)

An intensive short course on Digital Computer Techniques for process identification and control. This short course is intended for persons who have some background in the basic elements of process control and who are interested in learning about process identification and more advanced digital control methods, or in updating their knowledge in these areas. The course is built around a series of identification and controller design workshops, using a user-friendly, interactive, graphics-based software package running on VAX's or IBM PC's. For details, contact Dr. P. A. Taylor, Department of Chemical Engineering, McMaster University, Hamilton, Ontario, Canada, L8S 4L7 (416) 525-9140, ext. 4952. FAX (416) 522-0058.

Short Course

Computer Methods for Process Design and Optimization, Engineering Design Research Center, Carnegie Mellon University, Pittsburgh
(May 22-26, 1989)

This course deals with recent developments in the areas of process synthesis, retrofit design, operability and batch processing using computer methods based on nonlinear and mixed-integer programming and expert systems. The format of the course includes lectures, sample problems, demonstrations and hands-on workshops. The instructors of the course are Professors Larry Biegler, Ignacio Grossmann and Arthur Westerberg. For information please call (412)268-2207.

1989 American Control Conference, The Pittsburgh Hilton and Towers
(June 21-23, 1989)

The American Automatic Control Council will hold the eighth American Control Conference (ACC) on June 15-17, 1988 at the Pittsburgh Hilton and Towers, Pittsburgh, Pennsylvania. The conference will bring together people working in the fields of control, automation, and related areas from the American Institute of Aeronautics and Astronautics (AIAA), American Institute of Chemical Engineers (AIChE), American Society of Mechanical Engineers (ASME), Association of Iron and Steel Engineers (AISE), Institute of Electrical and Electronic Engineers (IEEE), Instrument Society of America (ISA), and the Society of Computer Simulation (SCS).

Both contributed and invited papers are included in the program. The ACC will cover a range of topics relevant to theory and practical implementation

of control and industrial automation and to university education in controls. Topics of interest include but are not limited to linear and nonlinear systems, identification and estimation, signal processing, multivariable systems, large scale systems, robotics and manufacturing systems, guidance and control, sensors, simulation, adaptive control, optimal control, expert systems, and control applications.

The organizing committee intends to arrange workshops to be held in conjunction with the 1989 ACC. Interested individuals should contact the Special Events Chairman, Michael K. Masten, (214) 343-7695, or the General Chairman.

(*NOTE*: Though the October 14, 1988 deadline has passed, the following information should be of interest to those individuals who wish to attend the ACC.)

CAST Area 10b is planning to sponsor or cosponsor a number of invited sessions at the 1989 American Control Conference. Chairs for these prospective sessions have been appointed and are now actively organizing them. A list of session titles follows. If you are interested in presenting a paper in an invited session, you should communicate with the appropriate chair or co-chair directly. One page abstracts of all prospective papers must be available to session organizers by October 14. Proposed AIChE Invited Sessions:

1. **Advances in Process Control** (possibly two sessions)

Evangelos Zafiriou
Department of Chem. & Nuclear Eng.
University of Maryland
College Park, MD 20742
(301) 454-5098

Jorge Mandler
Air Products & Chemicals
Box 538
Allentown, PA 18105
(215) 481-3413

2. **Robust Control**

Yaman Arkun
School of Chemical Engineering
Georgia Inst. of Technology
Atlanta, GA 30332-0100
(404) 894-2865

Manfred Morari
Department of Chemical Engineering
California Inst. of Technology
Pasadena, CA 91125
(818) 356-4186

3. **Control of Distributed Parameter Systems**

Vasilios Manousiouthakis
Department of Chemical Engineering
UCLA
Los Angeles, CA 90024
(213) 825-9385

4. **Applications of Artificial Intelligence to Process Control**

Ali Cinar
Department of Chemical Eng.
Illinois Inst. of Technology
Chicago, IL 60616
(312) 567-3042

Bradley Holt
Department of Chemical Eng.
University of Washington
Seattle, WA 98195
(206) 543-0554

5. **Control of Chemical Reactors**

Christos Georgakis
PMC Research Center
Lehigh University
Bethlehem, PA 18015
(215) 758-4781

6. **Decentralized Control**

Dominique Bonvin
Technisch-Chemisches-Labor
ETH-Zentrum
CH-8092 Zurich/Switzerland
01/256 31 13

Yaman Arkun
School of Chemical Engineering
Georgia Inst. of Technology
Atlanta, GA 30332-0100
(404) 894-2865

7. **Recent Advances in Adaptive Process Control**

Spyros Svoronos
Department of Chemical Engineering
University of Florida
Gainesville, FL 32611
(904) 392-9101

Duncan Mellichamp
Dept of Chemical & Nuclear Eng.
University of California
Santa Barbara, CA 93106
(805) 961-2821

8. **Advanced Distillation Column Control** (Jointly Sponsored w/ ISA)

Sten Bay Jorgensen
Department of Chemical Engineering
Technical University of Denmark
DK 2800 Lyngby, Denmark
(02) 88 32 88

Tom McAvoy
Department of Chemical & Nuclear Eng.
University of Maryland
College Park, MD 20742
(301) 454-4593

9. **Control of Biochemical Processes** (Joint w/ ISA)

Satish Parulekar
Dept. of Chemical Engineering
Illinois Institute of Technology
Chicago, IL 60616
(312) 567-3044

Karen McDonald
Dept. of Chemical Engineering
University of California
Davis, CA 95616
(916) 752-0400

10. **Control of Metals Processing**
(Jointly Sponsored w/ AISE)

William Tomcanin
Alcoa Laboratories
Aluminum Company of America
Alcoa Center, PA 15069
(412) 337-2942

For further information, please contact:

Professor Duncan Mellichamp (AIChE Society Review Chairman), Department of Chemical Engineering, University of California, Santa Barbara, CA 93106, (805) 961-3411; Professor Marija Ilic (Program Chairman), LEES, Bldg. 10-059, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, (617) 253-4682; Professor H. Vincent Poor (General Chairman), Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, 1101 West Springfield Avenue, Urbana, Il 61801, (217) 333-6449.

Foundations of Computer-Aided Process Design
(FOCAPD-89) Snowmass, CO
(July 9-14, 1989)

Jeffrey J. Siirola (Chairman), Eastman Kodak Company, P.O. Box 1972, Kingsport, TN 37662, (615) 229-3069 and Ignacio E. Grossmann (Co-Vice Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268- 2228.

The following is the tentative program for the meeting.

Nine sessions are planned. Conference themes include: Design Theory and Methodology, Artificial Intelligence, New Design Environments, Process Synthesis, Mathematical Techniques, Process Simulation and Analysis, Applications of Supercomputers, Chemical Product Design, and Future Outlook. See the special announcement elsewhere in this issue.

Session 1:

Keynote Address

Critical Issues in Design Theory and Methodology. Michael J. Wozny, Rensselear.

Session 2:

Artificial Intelligence in Design. Chairman: John C. Hale, DuPont.

Artificial Intelligence and Symbolic Computing in Process Engineering Design. George Stephanopoulos, MIT.

Computer-Aided Process Design Systems with Knowledge Base: Present and Future. Kiyoyuki Suzuki, Intelligent Technology Inc.

A Blackboard-based Architecture for VLSI CAD Tool Integration. Stephen W. Director, Carnegie Mellon.

Session 3:

Approaches to Chemical Process Synthesis. Chairman: David W. T. Rippin, ETH.

A Hierarchical Decision Procedure for the Conceptual Design of Chemical Processes. James M. Douglas, University of Massachusetts.

The Impact of MINLP Algorithms in Process Synthesis. Ignacio E. Grossmann, Carnegie Mellon.

Session 4:

Systems Analysis Tools for Chemical Process Design. Chairman: Henry M. Gerhardt, Amoco Chemical.

Nonlinear Systems Analysis in Process Design. Warren D. Seider, University of Pennsylvania.

Strategies for Simultaneous Solution and Optimization of Differential-Algebraic Systems. Lorenz T. Biegler, Carnegie Mellon.

Recent Developments in Methods for Finding All Solutions to General Systems of Nonlinear Equations. J. D. Seader, University of Utah.

Session 5:

Additional Chemical Process Design Issues. Chairman: H. Dennis Spriggs, Linnhoff-March

Recent Developments in Systematic Methods for Retrofit Process Design. Truls Gundersen, Norsk Hydro.

Progress and Issues in Computer-Aided Batch Design. G. V. Reklaitis, Purdue.

Session 6:

Process Design Environments. Chairman: Edward M. Rosen, Monsanto.

A State-of-the-Art Process Synthesis and Analysis Environment. Don Vredeveld, Union Carbide.

Integrated Process/Plant Design. Malcolm L. Preston, ICI.

Application of Advanced Architectures to Practical Chemical Engineering Design Problems. Gregory J. McRae, Carnegie Mellon.

Session 7:

Product Design. Chairman: Joseph D. Wright, Xerox Research Centre of Canada.

Designing Molecules Possessing Desired Physical Property Values. Kevin G. Joback, MIT.

Molecular Modeling for the Design of Pharmaceuticals. Robert Langridge, University of California - San Francisco.

Computing in CAR Product Design. Kenneth H. Huebner, Ford.

Session 8:

New Challenges in Process Design. Chairman: John D. Perkins, Imperial College.

Robust Solution of Flowsheeting Equation Systems. Ross E. Swaney, University of Wisconsin.

Design of Multipurpose Batch Plants with Multiple Production Routes. Iftekhar A. Karimi, Northwestern.

Systematic Synthesis of Separation Schemes for Azeotropic Mixtures. Michael F. Doherty, University of Massachusetts.

Simultaneous Process Synthesis and Control of Chemical Systems: Disturbance Rejection. Christodoulos A. Floudas, Princeton.

Design and Synthesis Methods for Polymer Processes. Michael F. Malone, University of Massachusetts.

Computer-Aided Analysis and Design in Polymer Processing. Andrew N. Hrymak, McMaster University.

Session 9:

The Future of Product and Process Design. Chairman: Jeffrey J. Siirola, Eastman Kodak.

Future Directions in Design and Design Environments. Arthur W. Westerberg, Carnegie Mellon.

Future Demands in Chemical Product and Process Engineering. L. E. Scriven, University of Minnesota.

Process Design – What Next? Roger W. H. Sargent, Imperial College.

Philadelphia AIChE Meeting
(August 20-23, 1989)

1989 International Conference on Parallel Processing, Pennsylvania State University
(August 8-12, 1989)

Pakers at this conference will describe recent advances on all aspects of parallel/distributed processing. These may include parallel/distributed logic circuits; impact of VLSI to parallel processor architecture; various concurrent-, parallel-, paper-, line-, or multiple-processor architectures; processor-memory interconnections; computer networks; distributed databases; reliability and fault tolerance; modeling and simulation techniques; performance measurements; operating systems; languages; compilers; algorithms; or various application studies.

The deadline for submitting papers is has passed, but CAST division members may be interested in attending the conference. For further details, contact: Dr. Peter M. Kogge, Mail Stop 0302, IBM Corporation, Route 17C, Owego, NY 13827, (607) 751- 2291. Please limit the length of your paper to about 20 double- spaced typed pages.

Computer Integrated Process Engineering (CIPE '89), Leeds, England
(September 25-28, 1989)

A major aim of the CIPE '89 conference is to review the field of advanced computer based technologies, with emphasis on integration, and to examine the problems of bringing together well-established applications packages to create the integrated process systems design environment. A second aim is to explore newer developments in hardware and software that specifically address issues relating to integrated design.

This call for papers invites contributions in the three linked fields of enabling technology, integration, and applications:

Enabling Technologies

- Mathematical and numerical methods
- Software engineering
- Graphics
- Databases
- Parallel processing
- Hardware architectures
- Man-machine interfaces

Integration

- CAD/CAE integration
- Management information systems
- Integration of design/control/ operation
- Computer-aided project management
- Decision support systems
- Computer integrated manufacture (CIM)

Applications

- Plant-wide systems
- Discrete/continuous systems
- Real-time applications
- Flexible production systems
- Operator training

Papers will be presented in sessions opened by a keynote speaker conducted by a chairman/rapporteur. It is intended that discussion of the papers will be an integral element of the meeting, and adequate time for this will be included in the program. All papers will be refereed.
Call for Papers – Timetable for Authors

October 1, 1988 Submission of 500-word abstract in English

December 1, 1988 Notification to authors of acceptance of abstract

March 1, 1989 Submission of paper for refereeing

July 1, 1989 Final submission of paper

Preprints of all papers will be distributed to conference participants approximately two weeks before the congress. Final proceedings, including updated papers, comments of session chairmen, and summaries of discussions will be published in the IChemE's Symposium Series and will be mailed to participants one month after the conference.

The conference is aimed at industrial and academic engineers and scientists engaged in computer-aided design, production, and development. The conference organization reserves the option to limit the number of participants to 180 on a first-come, first-served basis. Early registration is therefore recommended. A few places will be reserved for junior researchers at a reduced registration fee.

Please direct correspondence to: CIPE '89, Attn. Prof. C. McGreavy, The University of Leeds, Leeds LS2 9JT, England. Telephone: (0532) 332401. Telex: 556473 UNILDS G. Fax: 0532 332032.

San Francisco AIChE Meeting
(November 5-10, 1989)

See the Calls-for-Papers section of this newsletter. Note that the Calls are not complete. If you wish to present a paper in any of the sessions for which a Calls for Papers does not appear, please contact the session chairman. For further details, see "About This Issue."

IFAC World Congress, Tallinn
(1990)

Sub IPC4: Control of Chemical Processes and Processes for Natural Products Like Food, Wood, and Agriculture

Chairman: Mogens Kummel

Given below, with organizers listed in parentheses, are the planned sessions. Full papers need to be submitted by June 15, 1989. Interested authors should contact Professor Thomas J. McAvoy, University of Maryland, Department of Chemical and Nuclear Engineering, College Park, Maryland 20742-2111, (301) 454-2431.

Planned Sessions (first organizer is the session chairman):

1. Expert Control of Chemical Processes (McAvoy and Koivo)
2. Adaptive Control of Chemical Processes (Wittenmark and Bachmann)
3. Robust Control of Chemical Processes (Kantor and Skogestad)
4. Fault Detection and Safety (Bachmann and Takamatsu)
5. Batch Process Control (Rippin and Najim)
6. Plant-wide Production Control (Uronen and Pyzik)
7. Statistical Process Control (MacGregor and Morris)
8. Biotechnological Process Control (Halme and Staniskis)
9. Automatic Control Applications in Agriculture (Hashimoto)

New Orleans AIChE Meeting
(March 18-22, 1990)

Prospective session participants are encouraged to observe the following deadlines:

September 1, 1989: Submit an abstract of the proposed presentation to the session chairman.

October 1, 1989: Authors informed of selection and session content finalized.

January 1, 1990: Submit an extended abstract to be published for distribution at the meeting.

February 1, 1990: Final manuscript submitted to the session chairman.

Authors are reminded that under current AIChE meeting policy, the meeting booklet will contain only titles of the papers presented. However, a book of extended abstracts is distributed to attendees at the meeting. Moreover, authors may bring hardcopies of their papers for distribution at their session, and hardcopies or microfiche may be ordered at or after the meeting.

Area 10A: Systems and Process Design

1. **Artificial Intelligence Applications in Process and Product Design**. Babu Joseph (Chairman), Department of Chemical Engineering, Washington University, St. Louis, MO 63130, (314) 889-6076.

2. **Effective Platforms for User Interfaces**. Mohinder K. Sood (Chairman), Mobil R&D Corporation, PO Box 1026, Princeton, NJ 08540, (609) 737-4960.

3. **Design for Waste Accountability.** Chairman to be confirmed. Contact Michael F. Doherty, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003 (413) 545-2359.

4. **Process Design and Analysis.** Peter Douglas (Chairman), Department of Chemical Engineering, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada, (519) 885-2913.

Joint Areas 10A and 10C Sessions

1-2. **Hazard and Operability Analysis for Process Safety I and II** (Joint with Area 10C). Venkat Venkatasubramanian (Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4050.

For further information details concerning Area 10A sessions and scheduling, please contact Michael F. Doherty (Area 10A Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2359.

Area 10B: Systems and Process Control

1. **Control of Polymerization Reactors.** W. David Smith (Chairman), Polymer Products Department, E.I. DuPont de Nemours & Company, PO Box 80262, Wilmington, DE 19880-0262, (302) 695-1476.

2. **Industrial Applications of Process Control.** Jorge A. Mandler (Chairman), Research and Engineering Systems - MIS, Air Products and Chemicals, Inc., Allentown, PA 18195, (215) 481-3413.

For further information details concerning Area 10B sessions and scheduling, please contact Duncan A. Mellichamp (Area 10B Chairman), Department of Chemical and Nuclear Engineering, University of California, Santa Barbara, CA 93106, (805) 961-2821.

Area 10C: Computers in Operations and Information Processing

1. **Computer Aided Engineering.** S. Ganguly (Chairman)

2-3. **Application of Expert Systems in Process Operations I and II.** Peter Clark (Chairman), School of Chemical Engineering, Cornell University, Ithaca, NY 14853, (607) 255-8656 and Gary D. Cera (Vice Chairman), Mobil Research and Development Corporation, PO Box 1026, Princeton, NJ 08540, (609) 737-5299.

4. **Management and Reconciliation of Plant Data.** Mohinder K. Sood (Chairman), Mobil R&D Corporation, PO Box 1026, Princeton, NJ 08540, (609) 737-4960 and A. L. Parker (Vice Chairman), Shell Oil Company, PO Box 10, Norco, LA 70079, (504) 465-7459.

5. **Computer Networks.** Brice Carnahan (Chairman), Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, (313) 764-3366 and Norman E. Rawson (Vice Chairman), IBM Corporation - D051, 6901 Rockledge Drive, Bethesda, MD 20817, (301) 571-4445.

6. **Simulation for Process Operations.** Heinz A. Preisig (Chairman), Department of Chemical Engineering, Texas A&M University, College Station, TX 77843-3122, (409) 845-0386 and Ravi Nath (Vice Chairman), Union Carbide Corporation, 11111 Katy Freeway, Houston, TX 77079, (713) 973-5609.

For further information details concerning Area 10C sessions and scheduling, please contact Rajeev Gautam (Area 10C Chairman), UOP Molecular Seive Department, Tarrytown Technical Center, Tarrytown, NY 10591, (914) 789-3206.

Area 10D: Applied Mathematics and Numerical Analysis

No sessions are planned

For further information details concerning Area 10D sessions and scheduling, please contact Doraiswami Ramkrishna (Area 10D Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4066.

For further information concerning CAST Division sessions and scheduling, contact Jeffrey J. Siirola (Area Programming Chairman), ECD Research Laboratories, Eastman Kodak Company, P.O. Box 1972, Kingsport, TN 37662, (615) 229-3069.

San Diego AIChE Meeting
(August 19-22, 1990)

Chicago AIChE Meeting
(November 11-16, 1990)

The CAST Division is tentatively planning the following sessions at the Chicago meeting:

Area 10A: Systems and Process Design

1. Process Synthesis
2-3. Design and Analysis I and II
4. Batch Process Engineering
5. Design Methods for Solid-State Chemical Engineering
6. Design for Process Innovation

Area 10B: Systems and Process Control

1-2. Recent Advances in Process Control I and II

3. Nonlinear Control
4. Model Predictive Control
5. Artificial Intelligence/Neural Networks in Process Control
6. Process Control Education in the 1990s
7. Industrial Challenge Problems in Process Control

Joint Area 10B and Area 15C

1. Modeling and Control of Biochemical Processes

Area 10C: Computers in Operations and Information Processing

1-2. Advances in Optimization I and II

3-4. Parallel Computing I and II

5. Visualization of Complex Systems
6. Neural Networks

Area 10D: Applied Mathematics and Numerical Analysis

1. Mathematical Analysis of Complex Systems
2. Chaos
3. Applied Mathematics and Numerical Analysis
4. Applications of Unconventional Mathematics

For further information concerning CAST Division sessions and scheduling, contact Jeffrey J. Siirola (Area Programming Chairman), ECD Research Laboratories, Eastman Kodak Company, P.O. Box 1972, Kingsport, TN 37662, (615) 229-3069.

Area 10a

1. **Process Synthesis**. Christodoulos A. Floudas (Chairman), Department of Chemical Engineering, Princeton University, Princeton, NJ 08544, (609) 452-4595.

2. **Design and Analysis**. I. General. Michael F. Malone (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-0838.

3. **Design and Analysis.** II. Large Envelope Systems. Krishna R. Kaushik (Chairman), Shell Oil Company, P. O. Box 2099, Houston, TX 77252, (713) 241-2098.

4. **Batch Process Engineering**

Heinz A. Preisig (Co-Chairman), Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, (409) 845-0386 and Michael F. Malone (Co-Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-0838.

5. **Design Methods for Solid-State Chemical Engineering**. Michael F. Doherty (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2359.

6. **Design for Process Innovation.** Irven H. Rinard (Chairman), Department of Chemical Engineering, The City College of New York, Convent Avenue at 138th Street, New York, NY 10031, (212) 690- 6624.

Houston AIChE Meeting
(Spring, 1991)

Los Angeles AIChE Meeting
(Fall, 1991)

NEWS AND INFORMATION

Computer Aided Process Operations, Proceedings of the First International Conference on Foundations of Computer-Aided Processor Operations, Park City, UT, July 5-10, 1987. Edited by G. V. Reklaitis and H. D. Spriggs. 1988 viii + 720 pages, U.S. $ 223.75.

The objectives of the conference were: to define and discuss the problems of plant operations; report on the development and application of computing and computation tolls and techniques for solving these problems; and bring together leading academic and industrial representatives to promote increased future and interaction and cooperation in defining and solving operations problems.

CALL FOR PAPERS

CAST Sections at AIChE Annual Meeting, Houston Texas
(April 2-6,1989)

The CAST Division sessions at the Houston Meeting have been summarized in a previous section in this newsletter. Because the November 1, 1988 deadline for the selection of authors has passed, these Calls will not be repeated; readers are referred to Volume 11, No. 1 (April 1988) of CAST Communications for a listing. Based upon the deadlines for the Washington DC and San Francisco national meetings, the editor has reconstructed the remaining deadlines for the Houston meeting as follows:

March 1, 1989: Two copies of the final manuscript submitted to session chairman.

March 15, 1989: Session chairman submits manuscripts to New York in order to be made available at the Houston meeting.

April 2, 1989: If manuscript not submitted on March 15, 1989, bring it to Houston.

CAST Sessions at AIChE Annual Meeting, San Francisco
(November 5-10, 1989)

The CAST Division is planning the following sessions at the San Francisco meeting:

Area 10A: Computers in Process Design

- Process Design and Analysis I and II
- Advances in Process Synthesis I and II
- Design of Batch Processes
- Process Simulation in the Electronics Industry
- Integration of Process Design and Control (with 10B)

Area 10B: Computers in Process Control

- Advances in Process Control I and II
- Statistical Process Control
- Nonlinear Control
- Batch Process Control
- Integration of Process Design and Control (with 10A)
- Modeling Issues in Process Control

Area 10C: Computers in Operations and Information Processing

- Scheduling and Planning of Process Operations I and II
- Statistics and Quality Control I and II
- Artificial Intelligence and Expert Systems in Process Engineering

Area 10D: Applied Mathematics

- Progress in Applied Mathematics I and II
- Finite Element Applications in Chemical Engineering
- Applications of Bifurcation Theory to Chemical Engineering Systems

All of these sessions have been confirmed by the Meeting Program Chairman, John O'Connell (University of Virginia).

The names, addresses, and telephone numbers of the session chairpersons are given on the next several pages, as are brief statements of the topics to receive special emphasis in soliciting manuscripts for these sessions. Prospective session participants are encouraged to observe the following deadlines:

January 15, 1989: Revised session information. From area chairmen to meeting program chairman (MPC), Dr. John O'Connell (University of Virginia).

April 15, 1989: 1-2 page abstracts received by CAST co-chairmen of sessions.

May 2, 1989: Session chairman reviews Proposals to Present forms, selects speakers. Submits information to meeting program chairman (MPC). Authors notified of acceptance soon after this date.

June 2, 1989: Final session selection by meeting program chairman, who sends decisions to all programming chairmen.

June 23, 1989: Final program copy sent by session chairmen to meeting program chairman.

July 23, 1989: Final program copy sent by meeting program chairman to AIChE headquarters.

August 15, 1989: Extended abstracts submitted to session chairmen.

September 1, 1989: Extended abstracts submitted by program chairmen to AIChE headquarters.

October 1, 1989: Final manuscripts submitted to session chairmen.

October 16, 1989: Manuscripts submitted by session chairmen to New York in order to be made available for San Francisco meeting.

November 5, 1989: If October 16, 1989 deadline is not met, please bring manuscript to San Francisco in order to be available at the meeting.

The above listing of deadlines is the most extensive one published to date in CAST Communications. You can use it as a guide to probable deadlines for future AIChE meetings in which the CAST Division members participate as speakers.

Process Design and Analysis I and II.

These two sessions will focus on the application of techniques in process design and analysis to practical problems. Contributions are specifically invited in the following areas: large-scale optimization, evaluation of process options, detailed simulation of unit operations, design for safety and environmental impact, graphical methods, and visualization in design.

Chairman

K. R. Kaushik
Shell Oil Company
P. O. Box 2099
Houston, TX 77252-2099
(713) 241-2098

Co-Chairman

M. L. Preston
Imperial Chemical Industries
P. O. Box 7
Winnington, Northwich
Chesire, CW8 4DJ, England
UK (606) 704118

Advances in Process Synthesis I.

This session seeks contributions in all areas of process synthesis. Topics of interest include grassroot and retrofit advances in: design theory, reaction path synthesis, heat integration approaches and applications, reactor networks, separation synthesis, and synthesis for operability.

Chairman

Christodoulos A. Floudas
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263
(609) 452-4595

Co-Chairman

Don Vredeveld
Union Carbide Corporation
PO Box 8361
South Charleston, WV 25303
(304) 747-4829

Advances in Process Synthesis II.

Papers are solicited in all areas of chemical process synthesis, including new approaches for total process flowsheets, non-sharp complex and batch separation sequences, heat integration approaches and applications, and reaction path and reactor networks synthesis in both grassroot and retrofit situations.

Chairman

Christodoulos A. Floudas
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263
(609) 452-4595

Co-Chairman

Ross E. Swaney
Department of Chemical Engineering
University of Wisconsin
Madison, WI 53706
(608) 262-3641

Design of Batch Processes.

The session will focus on the general area of batch process design. The topics of interest include, but are not limited to, the design of multiproduct/ multipurpose plants; scheduling and/or planning considerations in design; design with uncertain process parameters and/or demands; intermediate storage design; availability and/or reliability analysis; retrofit design; design with resource/operation constraints; and flexibility in design.

Chairman

Iftekhar A. Karimi
Department of Chemical Engineering
Northwestern University
Evanston, IL 60208-3120
(312) 491-3558

Co-Chairman

Girish Joglekar
Batch Process Technologies, Inc.
P. O. Box 2001
West Lafayette, IN 47906
(317) 463-6473

Process Simulation in the Electronics Industry.

This session will emphasize the continuing role of chemistry and chemical engineering in the processes used to manufacture microelectronic devices. Papers are solicited from researchers and practitioners active in microelectronic manufacturing operations, e.g., manufacture of high-purity semiconductor materials, crystal growth, methods of purification, oxygen control in silicon, wafer fabrication, wafer processing, epitaxy, oxidation, lithography, diffusion, ion implantation, plasma processing, metallization, assembly, and packaging. Papers that address the other aspects of microelectronics fabrication based on chemical processes are also welcome. Papers on facilities preparation as well as utility supplies (de-ionized water, particulate-free

air, process gases, and chemicals) servicing microelectronics industry are also encouraged. Abstracts are due before April 15, 1989. Those interested in submitting a paper must submit a one- to two-page abstract. Authors' names and addresses should appear below the underlined title. Indicate the author who will present the paper with an asterisk.

Chairman

M. S. Bawa
Texas Instruments Inc.
PO Box 84, Mail Station 883
Sherman, TX 75090
(214) 868-7111

Co-Chairman

Narses Barona
Ethyl Corporation
451 Florida Street
Baton Rouge, LA 70801
(504) 359-2268

Integration of Process Design and Control

Contributions that report case studies of an integrated design of whole plants or parts of plants, and the associated control systems, are sought. This may include reports of any significant design modification that was made based on control-related considerations such as controllability, reliability, and safety of a plant, as well as robustness to anticipated disturbances or anticipated changes in the operating conditions. Theoretical contributions that focus on generic frameworks for handling the integration problem, may they be heuristic based or deep-knowledge based, are welcome.

Chairman

Heniz A. Preisig
Chemical Engineering
Department
Texas A&M University
College Station, TX
77483-3122
(409) 845-0386

Co-Chairman

Ahmet N. Palazoglu
Chemical Engineering
Department
University of California
Davis, CA 95616
(916) 752-8774

Advances in Process Control I and II.

Papers which demonstrate advances in process control or in the application of process control are invited. Relevant topics include: multivariable control, nonlinear control, robust control, adaptive and self-tuning control, plantwide control, model-predictive control, expert control systems, and statistical process control. Please send extended abstracts (500 words) to both co-chairmen. The abstract submission deadline is April 15, 1989.

Chairman

Ali Cinar
Department of Chemical
Engineering
Illinois Institute of
Technology
Chicago, IL 60616
(312) 567-3042
BITNET: CHECINAR@IITVAX

Co-Chairman

James J. Downs
Tennessee Eastman Company
PO Box 511
Kingsport, TN 37662
(615) 229-5318

Statistical Process Control.

This session will focus on the development and application of statistical process and quality control methods to chemical engineering problems. Topics for potential papers include applications to feedback control, process diagnosis, and fault detection. Proposals for tutorial papers will also be considered.

Chairman

P. Maurath
Procter and Gamble
Company
11530 Reed Hartman Hwy.
Cincinnati, OH 45241
(513) 530-3781

Co-Chairman

A. Katterson
Alcoa
Alcoa Technical Center
Alcoa Center, PA 15069

Nonlinear Control.

Papers are invited which demonstrate theoretical advances and novel applications in the following areas: exact and approximate linearization methods, nonlinear decoupling, observer design for nonlinear systems, nonlinear robust control, nonlinear optimal control, and discrete time control for nonlinear systems. Papers describing experimental control applications are also encouraged. Please submit an extended abstract (of no less than 500 words) to session chairman or co-chairman.

Chairman

V. Manousiouthakis
Department of Chemical
Engineering
University of California
Los Angeles, CA
90024-1600
(213) 825-2046

Co-Chairman

C. Kravaris
Department of Chemical
Engineering
University of Michigan
Ann Arbor, MI 48109-2136
(313) 764-1674

Batch Process Control.

Papers which demonstrate advances in batch process control theory or applications are invited. Topics of particular interest include: on-line optimization, parameter and state variable estimation, modeling issues, nonlinear model-based control, product property or quality control, and inferential control. Please send abstracts to Professor Bequette by April 15, 1989. Authors will be notified of acceptance decision by May 15, 1989. Acceptance for presentation obligates the authors to send the complete paper to Professor Bequette by October 15, 1989.

Chairman

John W. Hamer
Research Laboratories, B-82
Eastman Kodak Company
Rochester, NY 14650
(716) 477-3740

Co-Chairman

W. Bequette
Department of Chemical Engineering
Rensselear Polytechnic Institute
Troy, NY 12181
(518) 276-6377

Modeling Issues in Process Control.

This session has been organized to overview modeling approaches that are used in controller design. Relevant issues include the level of modeling 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. Please send an extended abstract (500 words) to both co-chairmen. Abstract submission deadline: April 15, 1989.

Chairman

Norman F. Jerome
Research Laboratories, B-82
Eastman Kodak Company
Rochester, NY 14650
(716) 477-2032

Co-Chairman

James Rawlings
Department of Chemical Engineering
University of Texas
Austin, TX 78712-1062
(512) 471-4417

Scheduling and Planning of Process Operations I & II

Topics of interest include new approaches and algorithms for the scheduling and production planning of multiproduct and multipurpose batch plants and of multiproduct continuous processes; long-range planning for capital investment; integration of planning and scheduling; and industrial experience with commercial software systems.

Chairman

Ignacio E. Grossmann
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2228

Co-Chairman

Peter Clark
School of Chemical Engineering
Cornell University
Ithaca, NY 14853
(607) 255-8656

Statistics and Quality Control I and II.

Chairman

Richard Mah
Chemical Engineering Department
Northwestern University
Evanston, IL 60201
(312) 491-3558

Co-Chairman

Gary Blau
Dow Chemical Co.
Engineering Research
1776 Bldg
Midland, MI 48640
(517) 636-5170

Artificial Intelligence and Expert Systems in Process Engineering

A general session dealing with the theory and application of artificial intelligence, knowledge-based and expert systems to process engineering. Emphasis will be given to papers describing applications that have followed through to delivery, and those incorporating new theoretical and methodological considerations. Papers dealing with knowledge representation, qualitative modeling, undertain reasoning, and the like are also welcomed. Areas of application may include product and process design, operations, and control. Authors of application papers should state the degree of completion and whether the system has been applied successfully.

Chairman

Mark A. Kramer
Department of Chemical Engineering
Room 66-542
Massachusetts Institute of Technology
Cambridge, MA 02139
(617) 253-6508
FAX: (617) 253-8000

Co-Chairman

Gary D. Cera
Mobil Research and Development Corporation
P. O. Box 1026
Princeton, New Jersey 08540
(609) 737-5299
FAX: (609) 737-5325

Progress in Applied Mathematics I and II

Papers are sought emphasizing applications of recent mathematical concepts and techniques; topics include analysis of simple systems displaying complex behavior, chaos, and new techniques for analysis of experimental data (time series, power spectrum) as well as mathematical modelling of chemical engineering processes.

Chairman

V. Balakotiah
Department of Chemical Engineering
University of Houston
Houston, TX 77004

Co-Chairman

R. Narayanan
Department of Chemical Engineering
University of Florida
Gainesville, FL 32611
(904) 392-9103

Chairman

Mike Doherty
Department of Chemical Engineering
University of Massachusetts
Amherst, MA 01003
(413) 545-2359

Co-Chairman

Julio Ottino
Department of Chemical Engineering
University of Massachusetts
Amherst, MA 01003
(413) 545-0593

Finite Element Applications in Chemical Engineering

Many of the newer areas of chemical engineering involve transport phenomena in micro-systems: crystal growth, chemical vapor deposition, electrochemistry, polymer processing, electronic component manufacture. This session emphasizes applications in which the role of the finite element method is important: problems with free and moving interfaces, graded meshes, and bifurcations.

Chairman

B. A Finlayson
Department of Chemical Engineering
University of Washington
Seattle, WA 98195
(206) 543-4483

Co-Chairman

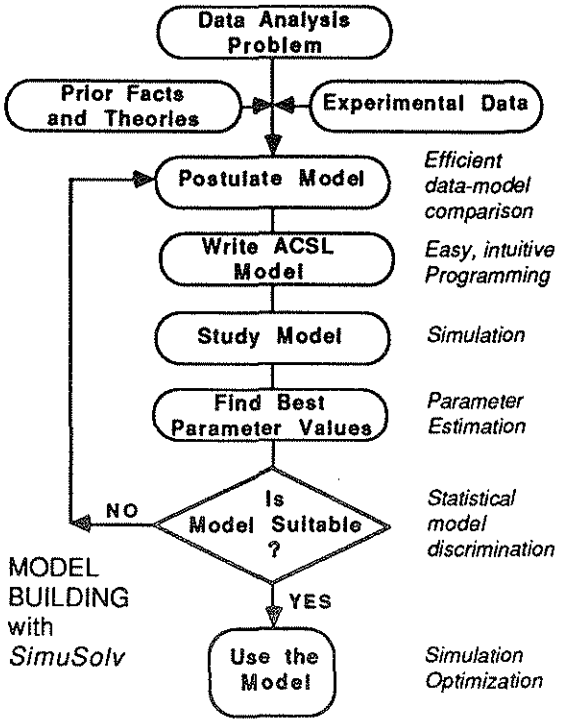
R. L. Sani
Department of Chemical Engineering
University of Colorado
Boulder, CO 80309-0424
(303) 492-5517

Applications of Bifurcation Theory to Chemical Engineering Systems

The theory of branching of solutions of nonlinear equations (bifurcation theory) is of great significance to the understanding of steady state (multiplicity) and dynamic (stability) characteristics of a diverse variety of chemical engineering systems. Papers are solicited emphasizing the combination of analytical tools with computational methods in this session.

SimuSolv*

MODELING AND SIMULATION SOFTWARE



CHEMICAL MODEL :

$$EO + NH3 \xrightarrow{K1} MEA$$

$$EO + MEA \xrightarrow{K2} DEA$$

$$EO + DEA \xrightarrow{K3} TEA$$

EO = Ethylene Oxide
NH3 = Ammonia
MEA = MonoEthanolAmine
DEA = DiEthanolAmine
TEA = TriEthanolAmine

KINETIC MODEL :

$$\frac{dMEA}{dt} = K1 * EO * NH3 - K2 * EO * MEA$$

$$\frac{dDEA}{dt} = K2 * EO * MEA - K3 * DEA * EO$$

$$\frac{dTEA}{dt} = K3 * EO * DEA$$

$$EO = EOIC - (MEA - MEAIC) - 2(DEA - DEAIC) - 3(TEA - TEAIC)$$

$$NH3 = NH3IC - (MEA - MEAIC) - (DEA - DEAIC) - (TEA - TEAIC)$$

SimuSolv MODEL (Partial):

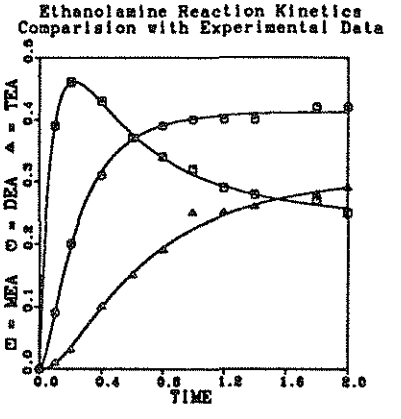
```
PROGRAM   ETHANOLAMINE REACTION
 INITIAL   $ 'INITIALIZE VARIABLES'
 END
 DYNAMIC
   DERIVATIVE
      dMEAdT  =  K1 * EO * NH3  - K2 * EO * MEA
      dDEAdT  =  K2 * EO * MEA  - K3 * EO * DEA
      dTEAdT  =  K3 * EO * DEA
      MEA     =  INTEG( dMEAdT, MEAIC )
      DEA     =  INTEG( dDEAdT, DEAIC )
      TEA     =  INTEG( dTEAdT, TEAIC )
      EO      =  EOIC - (MEA-MEAIC) ...
                 - 2(DEA-DEAIC) - 3(TEA-TEAIC)
      NH3     =  NH3IC - (MEA-MEAIC) ...
                 - (DEA-DEAIC) - (TEA-TEAIC)
   END
   TERMT(TIME .GE. TSTOP)
 END
END
```

Unmatched Capabilities for Mathematical Modeling

The SimuSolv computer program is designed to help the engineer develop and build mathematical models of physical systems. The philosophy of Simusolv is to enable the engineer to use the most sophisticated modeling techniques without having to become an expert in computational procedures. It features use of the continuous simulation language ACSL®, integration methods for stiff and nonstiff systems, constrained nonlinear optimzation capabilites, maximum likelihood parameter estimation and extensive graphics capabilites.

Typical Applications of SimuSolv are:

- Determination of **chemical and polymerization kinetics**
- Optimal **design and operation of reactor systems**
- Dynamic **heat and mass transfer studies**



For More Information Contact

United States and Canada
Mitchell and Gauthier Associates, Inc.
73 Junction Square Drive
Concord, MA 01742
508-369-5115

Europe
Rapid Data Ltd
Crescent House
Crecent Road, Worthing
West Sussex BN11 5RW
England
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AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

1989 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.		

Please send the completed form and supplemental sheets by April 3, 1989 to the CAST Division 2nd Vice Chairman, Professor G. V. (Rex) Reklaitis, School of Chemical Engineering, Purdue University, West Lafayette, IN 47907 (317) 494-4075..