

Computing and Systems Technology Division Communications



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CAST Division of AIChE 1993 Executive Committee

Elected Members

Past Chair

Ignacio Grossmann
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2228
Fax: (412) 268-7139
Email: D391GR99@CMCCVB.BITNET

Chair

Michael F. Doherty
Chemical Engineering Department
University of Massachusetts
Amherst, MA 01003
(413) 545-2359
Fax: (413) 545-1647
Email: MDOHERTY@ECS.UMASS.EDU

1st Vice Chair

W. David Smith, Jr.
E.I. duPont de Nemours & Company
Experimental Station
P.O. Box 80269
Wilmington, DE 19880-0269
(302) 695-1476

2nd Vice Chair

Rudolphe L. Motard
Washington University at St. Louis
Department of Chemical Engineering
One Brookings Drive, Urbauer Hall 208
St. Louis, MO 63130-4899
(314) 935-6072
Fax: (314) 935-4434
Email: MOTARD@WUCAPE@CAPE1.WUSTL.EDU

Secretary/Treasurer

Lorenz T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2232
Fax: (412) 268-7139
Email: D101LB01@CMCCVB.CC.CMU.EDU

Director, 1991-1993

James Deam
Monsanto Chemical Company
800 N. Lindbergh Boulevard
St. Louis, MO 63167
(314) 694-6061
Fax: (314) 694-6138

Director, 1991-1993

Mark R. Juba
Synthetic Chemicals Division
Eastman Kodak Company
Rochester, NY 14627
(716) 722-1417
Fax: (716) 722-4637

Director, 1992-1994

Gary D. Cera
Mobil R&D Corporation
Engineering Department
P.O. Box 1026
Princeton, NJ 08543-1026
(609) 737-5299
Fax: (609) 737-5325

Director, 1992-1994

James F. Davis
Department of Chemical Engineering
Ohio State University
140 West 19th Avenue
Columbus, OH 43210-1180
(614) 292-0090
Fax: (614) 292-3769
Email: davis@kcg11.eng.ohio-state.edu

Director, 1993-1995

Maria K. Burka
Chemical and Thermal System Division
Room 1115
National Science Foundation
Washington, DC 20550
(202) 357-9606
Fax: (202) 357-5184
Email: MBURKA@NSF.GOV

Director, 1993-1995

Stephen E. Zitney
Cray Research, Inc.
655-E Lone Oak Drive
Eagan, MN 55121
(612) 683-3690
Fax: (612) 683-3099
Email: SEZ@CRAY.COM

Ex-Officio Members

Programming Board Chair

Jeffrey J. Sirola
Eastman Chemical Company
Kingsport, TN 37662-5150
(615) 229-3069
Fax: (615) 229-4558
Email: SIROLA@KODAK.COM

Area 10a Systems and Process Design

Area 10a Chair

Lorenz T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA 15213
(412) 268-2232
Fax: (412) 268-7139
Email: D101LB01@CMCCVB.CC.CMU.EDU

Area 10a Vice Chair

Michael F. Malone
Department of Chemical Engineering
University of Massachusetts
Amherst, MA 01003-0011
(413) 545-0838
Fax: (413) 545-1647
Email: mmalone@ecs.umass.edu

Area 10b Systems and Process Control

Area 10b Chair

Ali Cinar
Department of Chemical Engineering
Illinois Institute of Technology
10 West 33rd Street
Chicago, IL 60616
(312) 567-3042
Fax: (312) 567-8874
Email: checinar@minna.iit.edu

Area 10b Vice Chair

James B. Rawlings
Department of Chemical Engineering
University of Texas
Austin, TX 78712-1062
(512) 471-4417
Fax: (512) 471-7060
Email: jbraw@che.utexas.edu

Area 10c Computers in Operations and Information Processing

Area 10c Chair

Gary D. Cera
Mobil R&D Corporation
Engineering Department
PO Box 1026
Princeton, NJ 08543-1026
(609) 737-5299
Fax: (609) 737-5325
Email: gdcera@engprn.mobil.com

Area 10c Vice Chair

Joseph F. Pekny
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907-1283
(317) 494-7901
Fax: (317) 494-0805
Email: pekny@ecn.purdue.edu

Area 10d Applied Mathematics and Numerical Analysis

Area 10d Chair

Yannis Kevrekidis
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263
(609) 258-2818
Fax: (609) 258-0211
Email: YANNIS@ARNOLD.PRINCETON.EDU

Area 10d Vice Chair

Hsueh-Chia Chang
Department of Chemical Engineering
University of Notre Dame
Notre Dame, IN 46556
(219) 239-5697
Fax: (219) 239-8366

AIChE Council Liaison

Bruce Finlayson
Department of Chemical Engineering
University of Washington, BF-10
Seattle, WA 98195
(206) 543-4483
Fax: (206) 543-3778
Email: Finlayson@cheme.washington.edu

Other Members

Publications Board Chair

Peter R. Rony
Department of Chemical Engineering
Virginia Polytechnic Institute & State Univ.
Blacksburg, VA 24061
(703) 231-7658
Fax: (703) 231-5022
Email: RONY@VTVM1

Associate Editor, CAST Communications

Joseph D. Wright
Xerox Research Centre of Canada
2660 Speakman Drive
Mississauga, Ontario, Canada L5K 2L1
(416) 823-7091
Fax: (416) 822-6984 (work)
(416) 332-1553 (home)
Email: WRIGHT.XRCC-NS@XEROX.COM

About This Issue

by Peter R. Rony, Joseph D. Wright,
and Jeffrey J. Sirola

Two speakers at the 1993 National AIChE Meeting in Miami Beach grace this Winter 1993 issue of CAST Communications. Computing in Chemical Engineering Award winner Warren Seider presents his CAST Division banquet address, "The Quantitative-Qualitative Dichotomy in Process Engineering" to all division members. Ross Taylor, who addressed the CACHE associates and trustees on Thursday night, contributes "Random Thoughts on User Interface Design for Engineering Software," a talk given to a standing-room only audience (with several colleagues rolling in the aisles). We dub Ross the "ChE humorist" for 1992.

At the CAST Executive Committee meeting, a new CAST policy was approved to have all speakers at CAST Division sessions provide "hard copies" of their visual aids to their audience (in addition to the manuscript that they provide to AIChE). This new policy is mentioned in the Call-for-Papers section, but we wish to stress its importance with an editorial comment here. Division members are encouraged to respond to this idea with comments directed either to the Chair of the CAST Division or to the editor of this newsletter. Our continuing objective is to improve the quality of our sessions. Your editor learned how to use several Microsoft Windows presentation packages during summer 1992. With both Microsoft PowerPoint and Lotus Freelance for Windows, he found it straightforward to produce printed sheets containing a group of 4 x one-fourth-size or 6 x one-sixth-size reductions of overheads, thus fulfilling the new CAST policy. Clearly, new applications software has reduced the burden of providing such visual aids to our colleagues.

The CAST Division is making a special effort to make more of its AIChE meeting program of relevance to practicing engineers. This goal will be emphasized at Spring meetings (in Houston and Atlanta) through topics directed at practical applications as well as session formats that include, for example, invited tutorials. Once again, the Division seeks responses from its members to this emphasis. The programming board was especially gratified by the turnout at the Area Programming meetings in Miami Beach. Your collective input has already begun to shape CAST programming, as evident in the listing published in this issue. To reinforce how important it is to the CAST Executive Committee that all division members feel comfortable in participating in programming activities, we wish to repeat the paragraph that we published in the Summer 1992 issue:

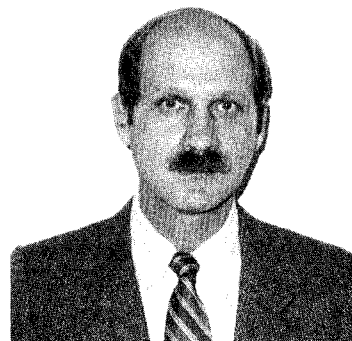
"Members of the CAST division programming board make a strong request for division members to participate in program planning meetings (there are four of them, for Areas 10a, 10b, 10c, and 10d) that are held in conjunction with the AIChE National Meeting in November. Specific times and meeting rooms are published in the meeting "green sheets" that are widely available at the registration area. Frequently, the meetings are during lunchtime. The CAST division seeks a broad spectrum of programming ideas and volunteers. Improved program quality and relevance, not only to division members but to all AIChE members, is important to us. If you cannot make the November meeting (the next one is in St. Louis), please submit suggestions to the CAST Programming Chairman, Jeffrey Sirola, anytime, by no later than two weeks before the meeting."

Your editorial board, Joe Wright and Peter Rony, sincerely thank the Computing and Systems Technology Division Executive Committee for

giving them plaques, at the Division Banquet in Miami Beach, in recognition of CAST Communications winning its second Marx Isaacs Award for Outstanding Newsletter of AIChE.

1992 Annual Report of the CAST Division

by Ignacio E. Grossmann



On behalf of the Computing and Systems Technology Division, I am very pleased to submit the 1992 Annual Report of the Computing and Systems Technology (CAST) Division. The mission of the CAST Division is to further the application of mathematical and computing principles in chemical engineering, particularly with respect to analysis, design, control, and operation of processes. This mission is achieved by pursuing three principal activities: AIChE session programming and specialist meeting organization, publications, and awards and recognition. The programming and meetings activity is supported through active collaboration with other divisions in the Institute as well as collaboration with other professional organizations with interests in computing and systems technology. The publications activity occurs principally through the Division newsletter, CAST Communications. The awards activity centers on three annual Division awards, with funding provided by industrial sponsors.

1992 Executive Committee and Elections

The CAST Division organizes its activities following its By-Laws and in 1992 performed its functions through the Division Executive Committee consisting of the following individuals with whom I had the great pleasure to work:

Prof. G.V. (Rex) Reklaitis, Purdue University, Past Chair

Prof. Ignacio E. Grossmann, Carnegie Mellon University, Chair

Prof. Michael F. Doherty, University of Massachusetts, First Vice-Chair

Prof. W. David Smith, Jr., E.I. DuPont de Nemours Co., Second Vice-Chair

Dr. Maria Burka, NSF, Secretary/Treasurer

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Dr. Mark R. Juba, Eastman Kodak Company, Director

Dr. Gary D. Cera, Mobil R&D Corporation, Director

Prof. James F. Davis, Ohio State University, Director

Dr. Jeffrey J. Sirola, Eastman Chemical Co., Programming Board Chair

Prof. Peter R. Rony, Virginia Polytechnic Inst., Publications Board Chair

Dr. Joseph D. Wright, Xerox Research Centre, Associate Editor, CAST Communications

The new officers elected in 1992 were Rudy Motard as 2nd Vice-chair, Larry Biegler as the new Secretary/Treasurer, and Steve Zitney and Maria Burka as the new Directors. We would like to extend to the new officers a

warm welcome. We would also like to express our sincere gratitude to Rex Reklaitis, our Past Chair, to Maria Burka the past Secretary/Treasurer, and to the two third year Directors, Mohinder Sood and Jim Deam.

Programming

Programming is the major activity of the Division which in 1992 was coordinated by the dedicated efforts of Dr. J. J. Sirola, the Programming Board Chair. The CAST Division programs at regular AIChE Meetings, organizes specialty conferences, and co-sponsors international meetings.

Regular Programming: Programming of sessions at regular AIChE Meetings occurs through four area committees: Systems and Process Design (10a), Systems and Process Control (10b), Computers in Operations and Information Processing (10c), and Applied Mathematics and Numerical Analysis (10d). Planning of sessions is done at least two years in advance. Priority is given to timely and relevant sessions. Also, considerable effort is expended by the Programming Board to insure that requested sessions are fully subscribed and completed.

There were 11 sessions sponsored by CAST at the New Orleans Spring Meeting, which were well attended. For the Fall Meeting in Miami, 24 sessions were organized by CAST, and 2 sessions were co-sponsored with Group 4. A poster session of the CAST Division also took place at that meeting. Also, posters of the CAST Division (which were donated by Kodak) were displayed at the entrance of the session rooms. For next year, 9 sessions sponsored by CAST have been approved for the Houston Spring Meeting. In the future, we will encourage CAST members to participate and submit more papers to the Spring meeting due to the reduction of sessions for the Fall meetings. For instance, next year no more than 20 sessions sponsored by

CAST have been approved for the Annual Meeting in St. Louis.

Specialty Conferences: Preparations are under way for the conference on Foundations of Computer Aided Process Operations that will take place in Mt. Crested Butte in July 1993. This conference is being co-sponsored by Area 10c. The conference on Foundations of Computer Aided Process Design, which is being co-sponsored by Area 10a, has been scheduled for the summer of 1994. CAST will also co-sponsor the International Process Systems Engineering Conference (PSE '94), that will take place in May of 1994 in Korea. Finally, Area 10b was involved in the organization of 7 sessions at the Automatic Control Conference in Chicago last June.

Publications

The Division newsletter CAST Communications appears semi-annually under the leadership of Editor Peter Rony and Associate Editor Joe Wright. CAST Communications was named the 1992 recipient of the Marx Isaacs Award for Outstanding Newsletter of AIChE. This is a significant achievement as this award was also given to our newsletter in 1990, the first year that the award was instituted. Peter Rony and Joe Wright should be recognized for their outstanding work in getting these awards. There are two new items that we have started in the last issue of CAST Communications. The first is a section entitled "Suggestions by CAST Members." The objective is to provide a mechanism by which CAST members can provide their input to the Executive Committee in the form of suggestions or comments on the activities of the Division. The second item is a new series that will describe academic research programs in CAST related areas at various universities. The last issue started with the program at Ohio State University. This issue features the program at

Purdue. Also in this issue, we start a new series on computing in industry. The objective is to describe developments in this area at various companies, and this issue describes the developments in Dow. Finally, there are plans for next year to prepare a special edition on Computing in Chemical Engineering in the Year 2000 that will appear in Chemical Engineering Progress in the late Fall of 1993. Our publications editor, Peter Rony, is coordinating these efforts on behalf of the CAST Division.

Awards

The 1992 recipients of the three CAST awards were: Professor Warren Seider of the Computing and Chemical Engineering Award (sponsored by Simulation Sciences Inc. and Dow Chemical), Mr. Greg Shinsky of the Computing in Practice Award (sponsored by Pergamon Press), and Professor Prodromos Daoutidis of the Ted Peterson Student Award, (sponsored by ChemShare Inc. and IBM). Details of the accomplishments of the awardees were given in the Summer 1992 issue of CAST Communications. The winners were recognized at the banquet of the CAST Division in Miami Beach.

Finances

The CAST Executive Committee approved last year a \$10 annual membership fee which became effective on January 1, 1993. This increase became necessary due to the increased expenses incurred in the production of the newsletter and to the limited funds that are available for undertaking new projects. It should be noted that the past membership fee of \$5 remained unchanged for more than 12 years. The new increase in the membership fee will allow CAST to provide several new services including the availability of a directory of CAST members.

Projects

In 1991 a new Long Range Plan was developed by the Division under the Past Chair, Rex Reklaitis. This plan involved the active participation of all the officers of the CAST Division. The plan identified areas where improvements are required and it suggested specific action items. The main area we concentrated on this year was membership of the Division. According to the Long Range Plan, the goal is to increase division membership at least 15% by 1996.

Since 1987, the Division has experienced very modest growth, and a slight decline for 1991 as shown by the following data (these are for the months of December of each year):

Year	Members
1987	1911
1988	1903
1989	1924
1990	1941
1991	1892

In August this year, CAST had 1992 members while in September it had 1885. This decrease is due to the annual update of division memberships that is performed by AIChE. Since during the next few months memberships are renewed, we will have to wait until the end of January to draw any definite conclusions on our performance in 1992.

This year we undertook a special effort for recruiting graduate students. We found out in 1991 that only 31 graduate students were members of the Division. In February 1992, we sent a mailing to all the Chemical Engineering departments in the U.S. soliciting names of graduate students working in the areas of design, control, applied mathematics, and computation. We received responses from 53 departments with 502 names

of graduate students. We used these names in a mailing in April with the help of AIChE (Joan Caputo, Gordie Ellis, Chris Burkett). We offered membership to CAST and to AIChE. As of October 30, 1992, 96 graduate students became new members of CAST; 52 of them also became new members of AIChE. We are most grateful for the very positive response by the graduate students and for the help from our academic colleagues.

In June, a special mailing was also prepared to contact local sections of AIChE to promote membership of practicing chemical engineers in the CAST Division. A flyer was also prepared and distributed at the Annual Meeting. Other projects that took place during this year included exploring the possibility of producing a CAST directory, sales of the newsletter to non-members, discussion on formats to ensure participation of speakers in the face of reduced sessions at the Annual meetings. Specific actions on some of these projects will be taken in 1993.

Finally, the CAST Division is pleased to announce that starting with the next AIChE Spring Meeting in Houston, authors will be strongly encouraged to bring copies of transparencies of their presentations. These will be provided free of charge to the attendees of the CAST sessions. It is hoped that this will be a useful service to the CAST membership and that it will help to improve the quality of the presentations.

Summary

In summary, CAST continues to be a very active Division of AIChE. The many events, services, and projects of the Division listed above are due to the outstanding efforts of the CAST Officers and Directors, as well as of many other members of the Division. We are most grateful for their help.

**New CAST Division Officers
Elected**

Rudolphe L. Motard

2nd Vice Chair



Rudy Motard holds a D.Sc. in Chemical Engineering, awarded in 1952, from Carnegie-Mellon University. His undergraduate degree was from Queen's University in Canada. He was on the faculty at the University of Houston for 21 years. He has been professor since 1978 and was the former chairman of the Department of Chemical Engineering at Washington University in St. Louis. Rudy has co-authored 34 publications, mostly on computer applications in chemical engineering. His pioneering work in chemical process simulation and other subjects has influenced both academic training and industrial practice. His current research interests include process synthesis, AI in process design, and process monitoring using wavelet transforms. He is a consultant to the AIChE process data exchange project (PDXI) at the University of Missouri. In Fall 1991, he received an award from the CAST Division in recognition of his professional contributions. Rudy served on the CAST Division Executive Committee in 1977-78 and 1985-87. He is a Fellow of AIChE.

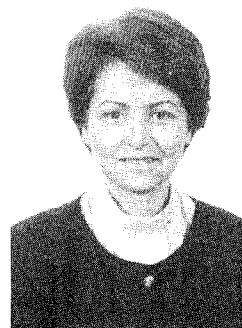
Lorenz T. (Larry) Biegler

Secretary/Treasurer

Larry Biegler is professor of chemical engineering at Carnegie-Mellon University, where he has taught since 1981. His chemical engineering education includes a B.S. from Illinois Tech, and M.S. and Ph.D. degrees from the University of Wisconsin. His research work includes process optimization with both steady-state and dynamic models, synthesis of chemical reactor networks, and process control strategies for nonlinear systems. In addition, Larry has contributed to teaching short courses on process modeling and optimization at Carnegie-Mellon, MIT, and for the AIChE. For the CAST Division, Larry has participated in Area 10a, 10b, and 10c programming sessions, is currently the Chair of Area 10a, and has chaired or co-chaired numerous technical sessions at annual and national AIChE meetings. He served as a CAST director from 1989-92. In addition, he is currently a CACHE trustee and served as CACHE secretary from 1990-92.

Maria K. Burka

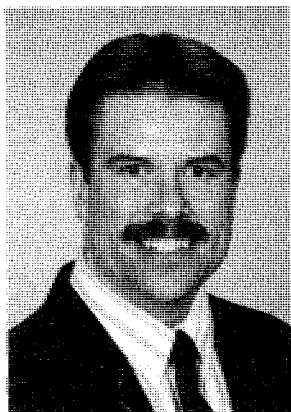
Director (1993-1995)



Maria, who has a B.S. and M.S. from MIT and both a M.A. and Ph.D. from Princeton University, is currently a program director for the Chemical Reaction Processes program at the National Science Foundation. The program funds basic and applied research in the areas of controls, design, polymerization, and reaction engineering. Previously, she was an environmental scientist at the Environmental Protection Agency, involved in research programs dealing with controlling NO pollution from stationary sources and pollutants from oil shale processing. Prior to that position, Maria was an Assistant Professor in the Department of Chemical Engineering at the University of Maryland at College Park. She is a member of AIChE, the CAST Division, AAUW, SWE, and Sigma Xi. For the past five years, from 1988-1992, she was the Secretary/Treasurer of the CAST Division. She has also served on the AIChE Nominating Committee.

Stephen E. Zitney

Director (1993-1995)



Stephen E. Zitney joined Cray Research in June 1989 as a Senior Chemical Engineer. As a member of the Chemical Research and Engineering Group, his research activities are focused on the development of new strategies for exploiting high-performance computing in steady-state and dynamic process simulation, optimization, large-scale separation systems, and process modeling for environmental applications. Stephen's other R&D interests include sparse matrix methods and parallel programming techniques.

Stephen earned a B.S. double degree in Chemical Engineering and Engineering and Public Policy from Carnegie-Mellon University in 1983. He received M.S. and Ph.D. degrees in 1986 and 1989, respectively, from the University of Illinois at Urbana-Champaign in the field of Chemical Engineering.

Stephen has authored or co-authored several technical publications and conference contributions on supercomputing strategies for chemical process engineering. Through his involvement with the CAST division of the AIChE, Instrument Society of America, Industrial Computing Society, and the Supercomputing Activity Group of SIAM, he actively promotes the use of

high-performance computing in the chemical science and engineering community.

CD-ROMs and Document Display Software

by Peter R. Rony

Your editor would like to share with Division members some thoughts about a number of computer-related items that have come to his attention since the last issue of this newsletter.

CD-ROM Publishing in Chemical Engineering

As a consequence of a presentation made by Professor Mike Cutlip, the new chairman of CACHE, at the spring trustees meeting, and a significant "multimedia" effort being initiated at his university (Virginia Tech, College of Engineering), CD-ROMs became so interesting that your editor is now the chairman of a newly formed (August 1992) CACHE ad hoc task force on CD-ROM Technology.

The first objectives of the task force were (1) to produce at least one demonstration chemical engineering CD-ROM and (2) to both demonstrate it and make several presentations about anticipated task force activities at the 1992 Miami Beach National AIChE meeting. On October 23, 1992, Nimbus Information Systems in Charlottesville, Virginia kindly provided the blank disc, the equipment, and the labor to produce CACHE CD-ROM #1, a single, "one-off" CD-ROM disc. CACHE publicly thanks them for their kind assistance.

The blank disc cost \$40, but the apparatus currently costs between \$7000 and \$12000, with prices expected to decline rapidly within the next several years. Within five years, most of you will have the

organizational capability to make your own CD-ROMs based upon \$5 blanks and "personal CD-ROM makers" that cost in the neighborhood of \$1000 plus hard disk. A very large hard disk, about 1.6 Gb, is required.

Do any readers know of other ChE software stored on a CD-ROM disc prior to October 23, 1992? If not, then CACHE CD-ROM #1 may have historical significance as the first ChE CD-ROM, or at least the first ChE educational CD-ROM. Hundreds, if not thousands, will follow in chemical engineering before the end of the century.

CACHE will continue to test the CD-ROM waters and, within about a year, will likely enter the business of creating custom CD-ROM discs for the chemical engineering educational community. Even today, the economics are attractive: after paying \$1000 in "mastering" costs and \$250 in "pre-mastering" costs, an organization can create its own CD-ROM discs for only \$2.00 each in minimum quantities of 200, and less for larger quantities. For 200 CD-ROMs, the per-CD-ROM cost is \$8.25; for 1000 CD-ROMs, the cost is only \$3.25 or less. Each CD-ROM stores as much as 640 Mb of information! Members of the CAST Division are invited to convey their perceptions about this technology to this newsletter.

The fly in this rosy ointment, to mix metaphors, is the compelling fact that most ChE professionals still do not have a CD-ROM drive in their PCs. We have the proverbial "chicken-and-egg-situation." What to do? These arguments were presented to Mark Rosenzweig, Editor-in-Chief of Chemical Engineering Progress (CEP) during the Miami Beach National Meeting, who wrote an editorial for the December 1992 issue. Of special interest is his description of the fact that the preprints for the first Separations Division Topical Conference weighed nearly six pounds, and came to almost 1200 pages.

Further, "these preprints represented less than 15% of all the presentations at the Miami Beach meeting. Preprints of all the presentations would have meant at least a sixfold increase in the number of pages and heft."

A similar story, with a sadder conclusion, came recently in an October 15, 1992 letter from the co-chairmen of the Annual Pittsburgh Modeling and Simulation Conference:

"...Costs of the Conference have steadily risen, but in the last several years, cost of publishing the Proceedings have skyrocketed. Although we have done our best to contain all of these costs in ways that we have previously communicated with you, we have not been successful."

"Since the Conference has always been a break even event on the basis of registration fees alone, we are now looking at registration fees in the \$300 range for a 2-day conference. This would be almost a 50% increase in the registration fee to continue the Conference. Therefore, we are informing you by this letter that no additional Modeling and Simulation Conferences will be held unless you explicitly hear from us to the contrary."

Perhaps the professional world needs fewer conferences, and perhaps some readers will shed few tears over the demise of this one. But the broader message is that rising publication costs increasingly threaten the ability of any professional organization to provide substantial printed information to its attendees. This is a global problem that transcends engineering.

Document Display Software: Display Postscript and MATHREADER

CD-ROMs to the rescue? Who knows? What form might they take? Your editor's initial guess was that the common denominator for the electronic

display of text, equations, and figures was some version of the Postscript™ standard. On November 12, he posed the question of Postscript-based document display software to two colleagues.

John Hassler, a faculty member at the University of Maine (HASSLER@MAINE) "ran a search on SIMIDX and only found (1) in TXTUTL - GETPSTXT.ARC (Convert Postscript to ASCII), and (2) in VENTURA - PSUTILS.ARC (Postscript utilities - no further description). I am sure such utilities must exist, perhaps as part of a word processor or Desktop Publishing package, but I don't know of any."

Dr. P. Kip Mercure (76067.432@CompuServe.COM), a colleague in the Camille Products group at The Dow Chemical Company, conveyed the following information:

"One of the problems is providing a reader so that all platforms can access the document. One possibility would be Wolfram Research's Mathematica™ program. They distribute a public domain program called MATHREADER to read Mathematica notebooks. I have versions for the Macintosh and the IBM PC. Since Mathematica is sold for a wide variety of platforms, I imagine that they have MATHREADERS for those platforms as well. The Mathematica notebooks can have platform independent text and images. I do not like the format of their equations in the body of text, but a more standard equation format could be done via the graphics. I DO like the general notebook format, AND you can do an index in Mathematica! If you don't use bitmaps, the mixture of text and graphics will probably be the problem."

Kip then sent a message to developers of Mathematica:

"Subject: MATHREADERS

A colleague and I are considering the possibility of publishing on CD-ROM. We are investigating machine

independent formats that would be usable across many platforms. The biggest problem seems to me to be mixing text and graphics. One possibility would be putting our articles in Mathematica™ notebooks and using the MATHREADER program to allow access from various platforms. I think that I have MATHREADER for Macintosh and IBM PC. On what platforms do you distribute MATHREADERS? What are the conditions for redistributing MATHREADER, say on CD-ROM? Regards, P. Kip Mercure"

The response was as follows:

"From: INTERNET:pkatula@wri.com

Subject: Mathematica Support

MathReader is available for the Macintosh, and Microsoft windows. It should be available for X some time after the X windows frontend is released. It is not currently available for the NeXT for some odd reason, though it should be easily possible. You may wish to contact Theo Gray at theodore@wri.com to ask him if this will soon be available for the NeXT. I am going to forward this message to John Cochrane regarding the legal matter of distributing MathReader on a CD ROM. He should be able to help you with that issue...Chris Rogers"

A definitive response came immediately from Wolfram Research:

"From: INTERNET:jhc@wri.com

Subject: MathReader

Cc: kevinr@wri.com

Wolfram Research allows MathReader to be redistributed for non-commercial purposes (i.e., not to be resold). If you are going to distribute your CD-ROM free of charge, you may redistribute MathReader in its entirety without any further interaction with Wolfram Research. If you plan to sell your CD-ROM, additional permissions need to be granted. Please contact me with details about your CD-ROM, and I'll be

happy to take care of this for you.
Sincerely, John Cochrane"

Adobe Acrobat

"Corporations are interested in electronic archival reports; corporate documents already might be saved for 50 years. My suspicion is that paper and microfiche are the current media in most places, but obviously it would be better to have something that is computer based. I know of individuals who considered Display Postscript, but they thought that the storage memory requirements would be too high. They are investigating storing in native format (i.e. Macintosh Word, Pagemaker, etc.) in conjunction with filter software from a company whose name escapes me now. The problem with this in the academic world is that the filter software is not free.

"As an experiment, I worked with chapter 1 of a typewritten document. The file sizes were:

MacWrite (original file): native – 48K,
compressed – 32K

Mathematica (images and text in Display Postscript): native – 202K,
compressed – 58K

So, if you are using an archiving utility the difference in size is not significant.

"I note that Adobe Systems has introduced a family of products to read documents in a mixed environment of Macintosh, Microsoft Windows, DOS, and Unix platforms. The products will be called 'Acrobat,' and are supposed to work with documents, photographic images, illustrations, graphs, and charts in a 'Portable Document Format.' Regards, P. Kip Mercure"

Adobe Acrobat? If you have been reading the trade journals starting in November 1992, you likely read the pre-release publicity about this product scheduled for release during 1993. In the February 1993 issue of Byte magazine, Rich Malloy's article, "COMDEX: Bigger Than Ever" (pages 41-42) selects the "best of show" as:

"And finally, we had to choose the Best of the Best, our Best of [COMDEX] Show Award. This honor was won easily by Adobe's Acrobat technology. We see this technology as having a far-reaching impact on the world of personal computing. If Acrobat delivers what Adobe says it will, it should touch the lives of every PC user. By helping to cut the wasteful use of paper, it should also help preserve resources, thereby touching the lives of everyone on the planet."

Purchasing CD-ROM Drives

Be careful when you purchase your first CD-ROM drive. An inexpensive drive, for under \$300, may become immediately obsolete. You may need a "multisession" CD-ROM drive that is capable of playing a CD-ROM that has several directories distributed throughout the disc, not a single directory at the beginning. A timely article by Jon Udell, "Start the Presses," in the February 1993 issue of Byte magazine (pages 116-134) offers the following summary advice in the sidebar, "Buying a CD-ROM Drive" (by Tom Halfhill):

"Here's the bottom line. If you need a CD-ROM drive to access static information—encyclopedias, technical manuals, reference books, and so on—you can get by with an inexpensive single-speed drive without XA or multisession support. For multimedia CD-ROM applications involving sound and animation, consider a dual-speed drive for best throughput. If you anticipate using Photo CD at all, you'll need at least an XA-ready single-session drive. For serious Photo CD work, settle for nothing less than a dual-speed drive with full XA and multisession capability."

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Dr. J.F. MacGregor & Dr. P.A. Taylor

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Dr. J.F. MacGregor and Dr. P.A. Taylor are professors in the Department of Chemical Engineering, McMaster University, Hamilton, Ontario, Canada. Both lecturers are recognized experts in the areas of process identification and control. They publish extensively in these areas, and consult for a wide variety of chemical and process industries throughout North America.

The number of participants is strictly limited. To ensure a place, please register as early as possible, preferably prior to April 12, 1993. For more information contact Dr. Paul Taylor at Tel. (416) 525-9140 (Ext. 4952) FAX (416) 521-1350 or write to: APC Course, P.O. Box 65516, Dundas Postal Outlet, Dundas, Ontario, Canada L9H 6Y6

Articles

The Quantitative-Qualitative Dichotomy in Process Engineering

by Warren D. Seider, Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA, 19104-6393



Introduction

As the field of chemical engineering progresses in step with the methods of mathematical analysis, most chemical engineers are carrying out more quantitative analyses, facilitated by high-speed computers, and involving detailed mechanisms that explain more complex phenomena. In parallel, however, several methods of qualitative analysis are also achieving a high level of mathematical rigor. These include order-of-magnitude analysis, fuzzy logic, and simulation by qualitative differential equations. Since, the latter are being applied with increasing frequency, it seems appropriate to consider the future roles of both quantitative and qualitative analyses in chemical engineering, and particularly in process engineering where uncertainties play an important role.

In the design stage, as in the simulation of an existing chemical process, the role of precise process models is often at issue. Questions such as: "How much precision is necessary?" or "How precise?" are

regularly considered. For example, when designing a separation train, more recent models for distillation account for two liquid phases on the trays, as shown schematically in Figure 1. Designers should ask the question: "How important is it to consider these details in an algorithm for process synthesis?" This question is difficult to answer in the design stages. Yet, the wrong answer could lead to a poor design or an unsophisticated design that is less profitable.

Two trends are appearing. These can be associated roughly with two schools of practice. In the first school, faster computers and larger memories are leading to more rigorous models that better represent the behavior of physical processes. As an example, process engineers are developing detailed finite-element models to describe the fluid mechanics and heat and mass transfer in the Czochralski crystallizer illustrated in Figure 2. The models are representing, with improving accuracy, the crystal diameter as the heating rate, pulling velocity, and rate of crystal rotation

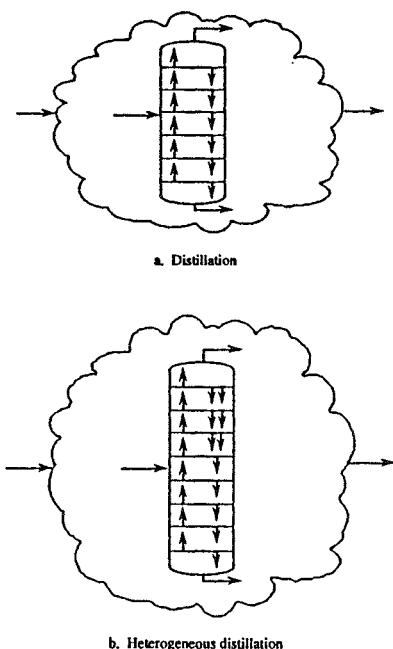


Figure 1: Separation train synthesis problem involving nonideal liquids: "How important is it to account for the second liquid phase?"

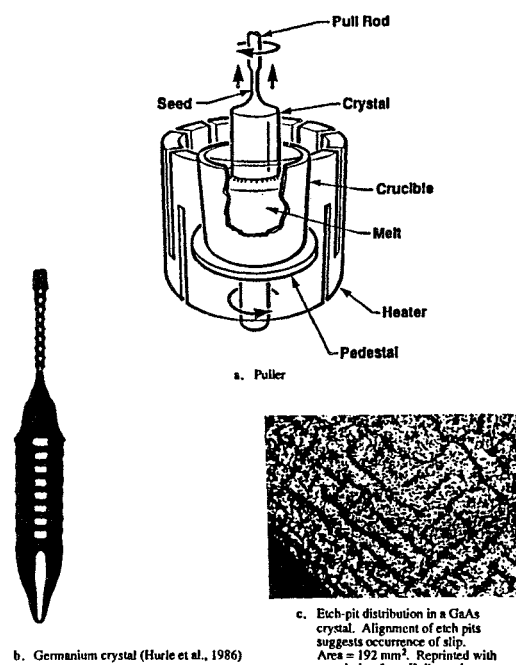


Figure 2: Czochralski crystallization

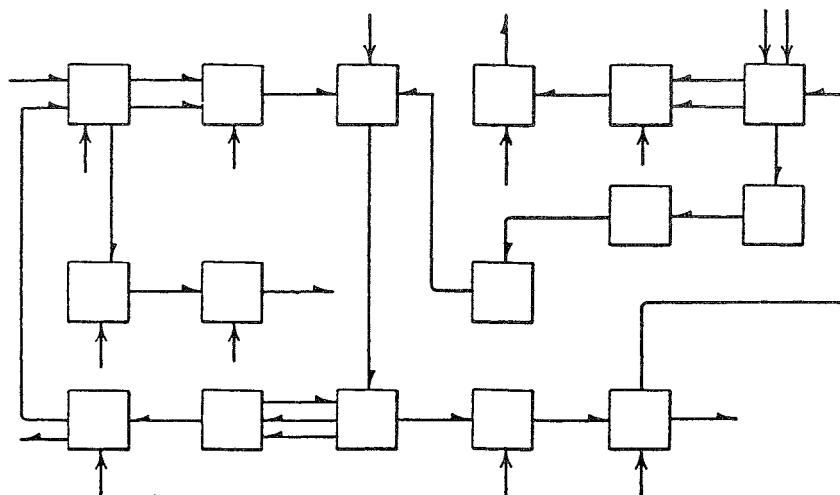


Figure 3: Process flowsheet showing the flow streams between the processing units

are varied. In the second school, on the other hand, faster computers and larger memories are stimulating the growth of models for very large systems; for example, to optimize refineries, and to calculate the concentration of CO_2 in the global atmosphere. When optimizing a large chemical process, a small portion of which is illustrated in Figure 3, the details of each processing unit are often less important. Often less *quantitative* (more *qualitative*) models are appropriate for these applications.

School 1

The first school is comprised principally of engineering scientists, applied physicists, physical chemists, and the like. These persons have concentrated on the development of macroscopic models, e.g., using the first and second laws of thermodynamics, and molecular reaction mechanisms. They are moving toward more fundamental models, e.g., involving statistical mechanics and free-radical reaction mechanisms, with many free radicals as intermediates at

low concentrations. Their experiments are carried out under carefully controlled conditions where *disturbances are unlikely*. Many compelling examples exist in the clean rooms of the microelectronics industry or the sterilized rooms of the pharmaceuticals industry. These models are often complex, involving sets of nonlinear differential equations, for which sophisticated applications of numerical methods are required to obtain solutions. In this respect, the pioneering text, "Applied Numerical Methods" by Carnahan, Luther, and Wilkes (1969), has been an important factor in the rapid development of sophisticated models over the past two decades.

School 2

On the other hand, the second school is comprised principally of process designers, control-system designers, operating engineers, plant managers, and others who perform related functions. These practitioners are usually concerned with, for example, optimizing the profitability, rejecting

unmeasured disturbances, and selecting from among many alternatives. They recognize that even the most sophisticated process models can be misleading in view of unexpected changes in the feed stock and product demand, and unmeasured disturbances during operation. Here, another pioneering text, the "Strategy of Process Engineering" by Rudd and Watson (1968), has played an important role in the rapid growth of analysis methods for large systems, while introducing the subject of uncertainty analysis.

Role of Qualitative Models

Before reviewing the methods of qualitative modelling, it is helpful to consider a key question: "What is the role of *qualitative* models?" Several observations are in order. To begin, it seems clear that qualitative (approximate) models should not be used to select from alternatives when more quantitative models are needed to describe the process being designed. As an example, when designing the fluidized-bed incinerator in Figure 4 to

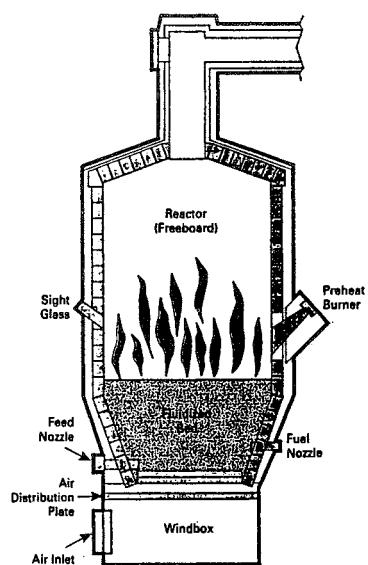


Figure 4: Fluidized-bed incinerator. Dorr-Oliver process. (Reprinted with permission from Mullen [1992])

achieve low levels of pollutants, such as NO_x and SO_2 , molecular models are inadequate. More detailed reaction mechanisms involving free radicals are needed to properly relate the concentration of the pollutants to the

residence time, the feed conditions, and the environment.

A less obvious danger lies in the application of models too approximate to identify the most promising designs.

Often these take advantage of complex physical and chemical interactions that lead to more economical processes. For example, consider the flash separators in Figure 5. In the manufacture of aniline, by the

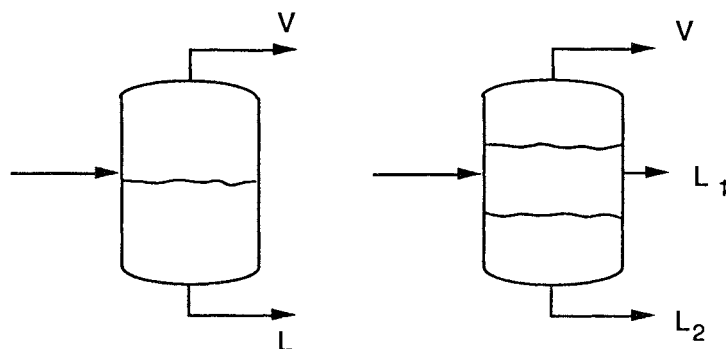


Figure 5: Two- and three-phase flash separators

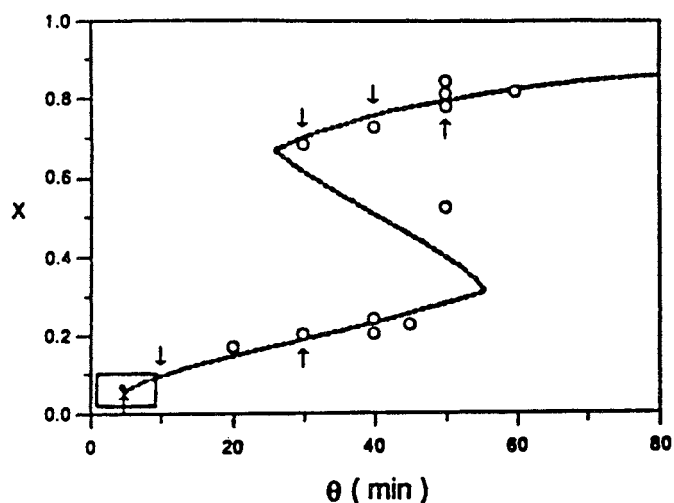


Figure 6: Steady-state conversion as a function of residence time in a CSTR for the emulsion polymerization of methylmethacrylate. (○) Data of Schork (1981), (●) Hopf bifurcation, (↑) dynamic simulation point, (---) unstable steady states. (Reprinted with permission from Rawlings and Ray (1987). Copyright 1987 Pergamon.

hydrogenation of nitrobenzene, Clark (1990) describes the advantages of operation within a small window of temperature and pressure in which a water phase can be decanted. Such a phase split can remove, or sharply reduce the need for a distillation tower to dehydrate the liquid product.

There is, however, a related caution. Some models can be too quantitative, providing numerical results that are too voluminous to draw attention to faults that occur during operation.

Still another danger occurs when approximate models miss regimes involving unstable steady states; that is, regimes characterized by hysteresis, periodic operation, and strange attractors. Often, these are the best economically and can be stabilized with modern, computer-based control systems. As an example, the data of Schork (1981) in Figure 6 for the emulsion polymerization of methyl methacrylate is in fine agreement with the population density model of Rawlings and Ray (1987). Stable steady states exist only at low residence times, with low conversions.

In the region of three steady states, beyond the Hopf bifurcation point, the high-conversion branch can be very attractive economically, but these steady states must be stabilized. Here, also, a related caution should be observed. Approximate models, with much nonlinearity, often incorrectly predict that such regimes exist. When predicted, it is important to confirm their existence, preferably with experimental measurements.

It also seems clear that misleading approximate models should not be used as the basis for decisions related to the global environment, even if insufficient computing power is available to model at the level of detail necessary. Large networks of parallel processors are engaged in calculating ozone concentrations on a global scale, but such models are necessarily limited by the quality of their kinetic mechanisms. Detailed reaction mechanisms, involving many free radicals at very low concentrations, are needed to predict the ozone concentrations recorded by a NASA spectrometer aboard the Nimbus 7 satellite, as illustrated in Figure 7, in

the view of the earth from over Antarctica. In my opinion, these calculations cannot be justified without a verified kinetic model, for they may otherwise predict misleading results. As a cautionary note, even the most quantitative models can be misleading! Their assumptions and underlying data must be checked carefully.

Qualitative Modeling

From the above, it seems clear that models are needed at the appropriate level of rigor. However, due to errors introduced by instruments, transmission lines, data-handling devices, among others, their parameters (e.g., thermophysical properties and kinetic constants) may be quite uncertain. Even the terms of the differential equations may be uncertain. Hence, it follows that *quantitative* differential equation models can be misleading.

Qualitative models, on the other hand, deal directly with uncertain parameters and data, and in some cases, with uncertain functionalities;

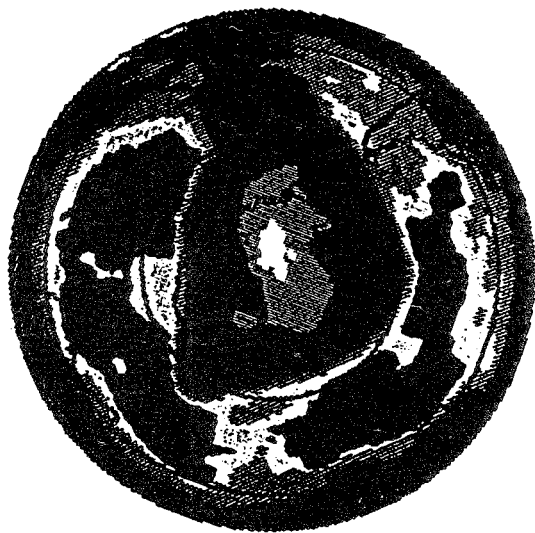


Figure 7: Ozone concentrations on October 5, 1989 measured by NASA spectrometer aboard the Nimbus 7 satellite. (Reprinted with permission from Zurer [1989])

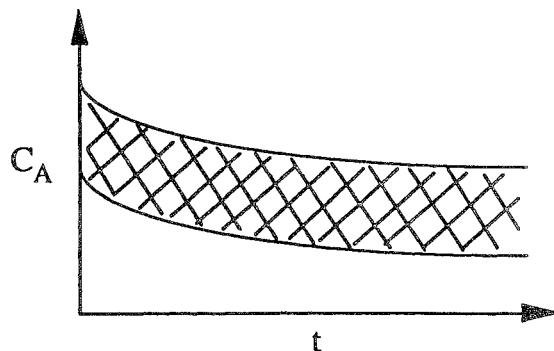


Figure 8: Bounded outlet concentration trajectories

that is, with incomplete knowledge. A traditional but limited approach to qualitative modeling places upper and lower bounds on the inputs and parameters of the differential models. Then, upper and lower bounds are computed on the dependent variables by solving the differential equations at intermediate and boundary values of the inputs and parameters. As an example, consider the mass balance for a CSTR in which species A is consumed by a second-order reaction:

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{Af} - C_A) - k C_A^2 \quad C_A \{ 0 \} = C_{A0}$$

When uncertainty is anticipated, bounds are estimated:

$$\begin{aligned} k^L &\leq k \leq k^U \\ C_{Af}^L &\leq C_{Af} \leq C_{Af}^U \\ F^L &\leq F \leq F^U \end{aligned}$$

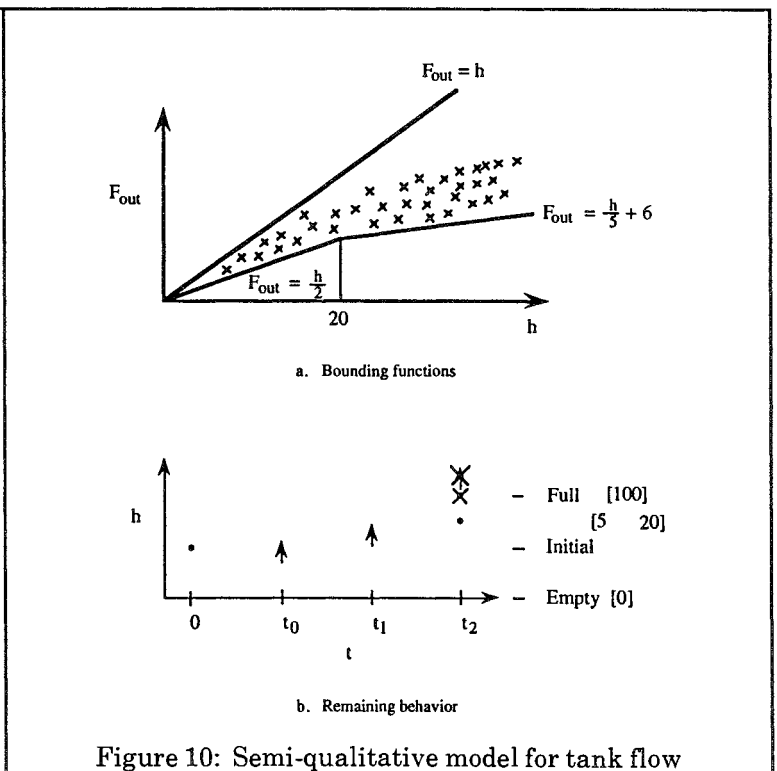
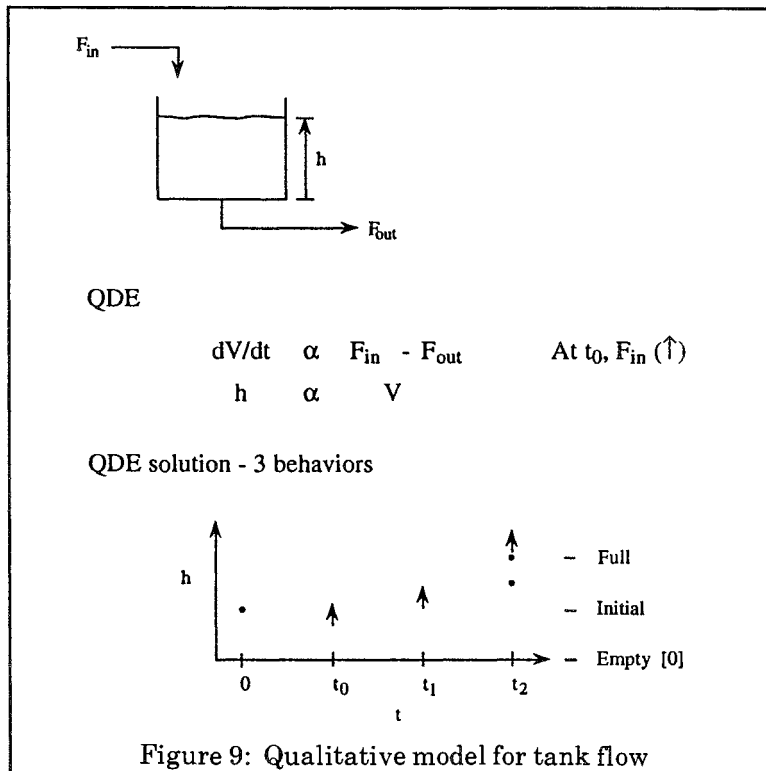
and a range of solution trajectories computed, with the upper and lower bounds as shown schematically in Figure 8. For dynamic systems, especially involving feedback control, stability and performance measures are checked by what is commonly referred to as *resiliency* analysis. For the design of systems in the steady state, the design is adjusted until all outputs satisfy the process constraints is a so-called *flexibility* analysis.

A more recent approach begins with variables and parameters that are higher than, lower than, or at *landmark* values, and are increasing, constant, or decreasing, but have no numerical values. In this environment, the differential equations reduce to qualitative differential equations (QDEs). For example, for flow in and out of a tank, the QDEs are shown in Figure 9. Here, a QDE solver, QSIM (Kuipers, 1986), solves for the three possible dynamic responses, known as *behaviors*, beginning with a partially full tank and an increase in F_{in} at t_0 . At intermediate times, t_1 , h is increasing in all of the trajectories. The

trajectories arrive at three final states at t_2 , overflow (\uparrow), steady full, and steady at intermediate h . These are the only three behaviors for the disturbance involving an increase in F_{in} .

When it is desired to eliminate unrealistic behavior, a more quantitative model can be generated by placing numerical bounds on the variables and introducing bounded functionalities. For tank flow, this could involve the introduction of experimental data to describe $F_{out} = f\{h\}$ with upper and lower bounds as illustrated in Figure 10. Then, the upgraded NSIM program (Kuipers and Berleant, 1988) can restrict the behaviors as shown in that plot. Note that only one behavior remains, with $5 \leq h \leq 20$ at t_2 . For this simple system, as the upper and lower bounds are reduced to $F_{out} = 1.2\sqrt{h}$ the behavior is known exactly (quantitatively).

Qualitative and semi-qualitative models, when solved using QSIM and NSIM, show excellent promise for the diagnosis of faults during the operation



of chemical processes (Vinson and Ungar, 1992). Here, the branches of the behavior trees, created by QSIM and NSIM, are traced to locate the possible causes of the faults. Qualitative and semi-quantitative models can also be used to prove that all behaviors of simple control systems achieve a stable response or a desired level of performance (Kuipers and Åström, 1991). This is accomplished without repeated solutions of differential equation models or the use of a linearized model in a conventional analysis for robustness.

In summary, the solutions of qualitative models permit reasoning based upon incomplete knowledge; that is, where, at best, parameters, inputs, and functionalities can only be bounded with confidence. The resulting conclusions are less quantitative, but apply to all behaviors that result from solving the QDEs.

Modeling Techniques

Given the relative ease of formulating and solving differential models with numerical parameters, inputs, and outputs, and the advantages of qualitative differential equations in accounting for uncertainties, the process engineer is challenged to combine these quantitative and qualitative formulations to develop realistic models.

On the quantitative side, in one widely-recognized approach, which does not directly account for uncertainty, terms are systematically removed from a complex differential model. For example, in fluid flow, one can begin with the fully-endowed Navier-Stokes equations, as presented in "Transport Phenomena" by Bird, Stewart, and Lightfoot (1960). Next, sensitivity analysis is applied to test the importance of the terms numerically. Today, finite-element meshes are generated automatically and solutions are computed for comparison with the fully-endowed

model. Note that this approach is implemented in an IBM PS/2 module prepared for students as a supplement to the fluid mechanics course (Fogler et al., 1992). The objective of this module is to teach the student to prepare *simplified* models.

On the qualitative side, the QDEs can be formulated initially with no bounds. For practical, nonlinear systems, their solutions involve a broad array of behavior. To gain resolution, bounds on parameters, and inputs, as well as envelopes to bound the functionalities, can be added gradually and systematically.

The Dichotomy in the Future

With the continuing development of faster computers with more memory, it seems reasonable to question whether the quantitative/qualitative dichotomy will become less significant. In my opinion, this will occur to some extent. However, more sophisticated models are likely to evolve that elucidate more complex phenomena which process engineers will seek to exploit in providing better products less expensively. As an example, return to the Czochralski crystallizer in Figure 2. More rigorous models can be expected to relate the instabilities at the meniscus (separating the liquid metal from its inert vapor surroundings) to the distribution of defects and dislocations in the crystal, as shown in the cross-section of the Si wafer in Figure 2c. Control systems that will utilize these advanced models (e.g., model-predictive controllers) should produce crystals contaminated with less faults.

It seems clear that the methods of quantitative analysis, coupled with carefully designed experiments, will continue to be most critical in the development of improved designs, operating strategies, and controls. But, qualitative models involving QDEs, order-of-magnitude analysis, and fuzzy logic will become better

defined and will play an important role.

In preparing to design the new processes and products in the future, young people entering the universities should question the relative importance of the principles associated with (1) *chemical processing*, i.e., thermodynamics, chemical kinetics, transport phenomena, statistical mechanics, and others, (2) *systems analysis*, i.e., nonlinear programming, decision theory, bifurcation theory, control theory, and others, and (3) *computer science*, i.e., languages, data structures, graphics, operating systems (windows), and others. Several observations are offered in the subsections that follow.

Computing Methodologies

It seems clear that process engineers must master the computing methodologies that are critical to the successful coordination of quantitative and qualitative models to achieve improved designs, operating strategies, and controls. However, when ranked in importance, as compared with the principles of chemical processing and systems analysis, several reservations are in order. In my opinion, the distinctions between computer languages are less important. Similarly, the optimization of data structures is less important, although inefficient data structures must be avoided when analyzing large-scale systems. Furthermore, efforts to utilize three-dimensional computer graphics and to apply parallel processing are less important.

Systems Analysis

It also seems clear that, to develop break-throughs in the processing of chemicals, next to carefully controlled experiments, the rate of progress depends on systems analysis to select near-optimal alternatives. This is a bewildering task as systems expand and encompass a vast number of

alternatives, only a few of which lie close to the optimum.

Conclusion

To do superior process engineering in the future (i.e., develop break-throughs in chemical processes and products), computing methodologies are critically important and systems analysis is crucial. At the heart, however, is chemical processing sophistication, i.e., the ability of process engineers to formulate and properly use quantitative and qualitative models, along with experimental data.

Acknowledgments

The helpful comments of Lyle H. Ungar and Evangelia A. Gazi, especially with regard to the qualitative aspects, are very much appreciated.

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Random Thoughts on User Interface Design for Engineering Software

by Ross Taylor, Department of
Chemical Engineering, Clarkson
University, Potsdam, NY 13699-5705



Introduction

Engineers want software that can solve their engineering problems. Given that technical excellence is essential, does the interface matter? The answer is most definitely in the affirmative. The last decade has seen major changes in the way we use computers and what we use them to do. In particular, the widespread use of personal computers and general purpose software such as word processors, spreadsheets, and tax preparation software (to identify just a few categories) has forever changed our expectations of how we want our engineering software to work. However, our willingness to use engineering software that does not come with a user friendly interface has decreased.

It could be argued that the most powerful of the software systems used by chemical engineers are flowsheeting packages. In their earliest incarnations, these programs could be run only after the user had created (using their favorite text editor) a long and complicated text file

containing the necessary input data. This approach, while it may once have been necessary, was never desirable and is no longer acceptable to modern users.

It is interesting to take a look back at the advertisements and publicity material of companies that create and market flowsheeting programs. Magazines like *Chemical Engineering Progress* (CEP) are a useful source of this kind of material. In times past, the emphasis in the advertisements was on the newer technical features of these programs. More recently, however, the advertisements and publicity material of these companies have focussed almost entirely on the new (usually graphical) interfaces that they have developed. For the user of these programs, these developments may have seemed to have been a long time coming but it must be recognized that interface development is a non-trivial task. Indeed, I would submit that it is much harder to write a good interface than it is to write the technical software that lies hidden behind the friendly faces.

It is, of course, relatively easy to write software that only the author must use. It is also straightforward to create software that others must use as long as they do not have to use it more than once. It is very difficult to write sophisticated software that others want to use again and again and again. What sets the one-off software package apart from one that is used repeatedly is that the latter has an interface that impresses users sufficiently that they are willing to use it again.

Those of us that are involved with the creation and support of technical software that others use know that it is necessary to devote a significant amount of time on the development of interfaces. Moreover, it is vitally important to get right what to the rest of the world appear to be trivial details. (For example, in what color should this message be displayed? Where should

the cursor go when some particular key is pressed?). Failure to get the details right will result in established users of your programs abandoning your software or will deny you the opportunity to gain new users at the expense of your competitors.

The purpose of this article is to present some thoughts on the design of interfaces for engineering software. I make no claim to be comprehensive. This article draws on the experiences of the author as one of the developers of *ChemSep*, a software system for the simulation of multicomponent separation processes. As part of my job as a university professor I have used and required students to use some of the commercially available flowsheet simulation packages. Some of the discussion below is drawn from experience with these programs.

Interface Design Philosophy

We believe that the interface is one of the most important, perhaps the most important, part of any software system. However, we have not yet defined what an interface is. For the purpose of this discussion, the interface is that part of the software package that allows the user to:

- (a) instruct the computer what engineering calculations are to be performed,
- (b) review the results of those engineering calculations,
- (c) as a result of (b), go back to (a) (and so we continue seemingly for ever).

We shall not consider interfaces where the user is not human (although sometimes we are tempted to wonder whether or not some of our users fall into that category anyway).

For the purposes of this discussion we shall consider two different groups of software users: novice and expert. Novice users have quite different requirements from experts. While it is usual to use general purpose software packages like word processors, editors,

and spreadsheets on an almost daily basis, very few users of engineering software use the same technical package every day. It is probably more common for engineers to make extensive use of one particular package over a short time but then not to use that package again for many months. In the meantime, our engineer has forgotten how to use the package (some of its important details at least) and will be a novice user for a short time again before graduating to the level of expert once more. The software developers themselves, are, of course, the ultimate experts; when compared to them, all other users are mere tyros.

Most of the users of the software that we develop are novices in every sense (not only are our students learning to use our software, they are also learning the subject that the software was created to help them study).

Our general philosophy when designing interfaces can be expressed in the form of a few simple rules:

Design for novices but allow for experts

Be consistent (with key and other assignments)

Keep it (the screen layout) clean

Software designers must be consistent with key assignments, screen design, use of colors, screen fonts, and so on. No user will appreciate inconsistencies in any aspect of your software. Colors need to be used with caution and software designers need to consider the needs of users who do not have color monitors (I suppose there are a few still around) or those who may be color blind. There is nothing like having a family member who is color blind to make you appreciate that their view of the world (and especially of PC games) can be different from yours.

Elements of Interfaces

The principal feature of all modern interfaces (and I use modern to mean current, fashionable, or temporarily desirable), no matter what computer

operating system they run under, is a window (Figure 1). Unfortunately, some windowing software systems (especially those of the graphical variety) have become so flexible that a good deal of control over the screen layout has been taken away from the software designer and placed in the hands of the user. What this means is that you can often see screens that have become so cluttered with overlapping windows (Figure 2) that it is impossible to see through or into any of them.

If one could look into one of these windows we might see some of the other building blocks of user interfaces.

- Spreadsheets
- Dialogue boxes (Figure 3)
- Lists
- Menus
- Illustrations (which might be graphs, charts or, in our industry, process flow diagrams)

Windows ...

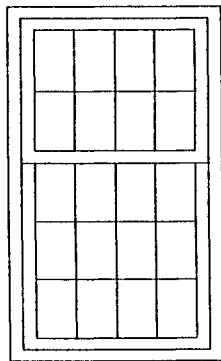


Figure 1: Windows ...

...Windows everywhere!

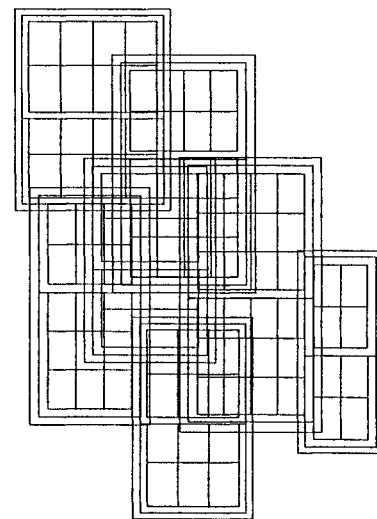


Figure 2: ... Windows Everywhere!

Menus

Menus are of two basic kinds; pull-down as shown in Figure 4 or Pop-up as illustrated in Figure 5. Of course, no software system has any value unless the main menu has sub-menus and the sub-menus have sub-sub-menus and so and so on... One of the problems that the software designer must face is how should the menus appear on the screen. Another issue is how do you move from one branch of the menu tree to another.

Imagine that you are a caterpillar on one of the lower branches of the menu tree in Figure 6 and you develop a craving for the leaves on one of the upper branches. It is certainly possible to crawl along the branch, up the main trunk and out along the branch with the tasty leaves. However, there is no doubt that you would be envious of the bird that can fly there directly. It is, therefore, essential to provide more than one way to get there from here.

It has become customary in PC software to move from one menu level to another using the <Return> and <Escape> keys. However, these key assignments, although extremely common, are not universally used. Some software employs other key combinations to perform the same functions. This might be satisfactory if the alternative key assignments were employed consistently throughout the program. Unfortunately, in some cases, they are not. In one simulation package both <Return> and the alternative work in some parts of the interface, sometimes only the alternative works, and sometimes only the <Return> key works!

Movement of the cursor in a menu tree should also be handled in a logical and consistent manner. The down key, for example, should always move the selection bar down. There is one commercial simulation program where the down arrow sometimes moves the selection bar down, on other occasions it causes a new option to be displayed.

Menus should wrap around at the ends. For example, depression of the down key when the cursor is located on the last item in a vertical menu should result in the selection bar jumping to the first item in the menu. Menu items should be selectable either by pressing the <Return> (or other consistently used) key when the selection bar is located or by pressing either a highlighted or the first character in the option name. Menus may need their exit clearly marked (preferably in addition to the standard <Escape> route).

The inconsistent use of key assignments is irritating at best and if we had just one request of other software designers it would be to get rid of unfamiliar key assignments in favor of something more conventional.

Menus should have a memory. That is, when you return to any menu the cursor should be located in the position it last occupied. In too many software packages the menus forget where they

Dialogue Boxes

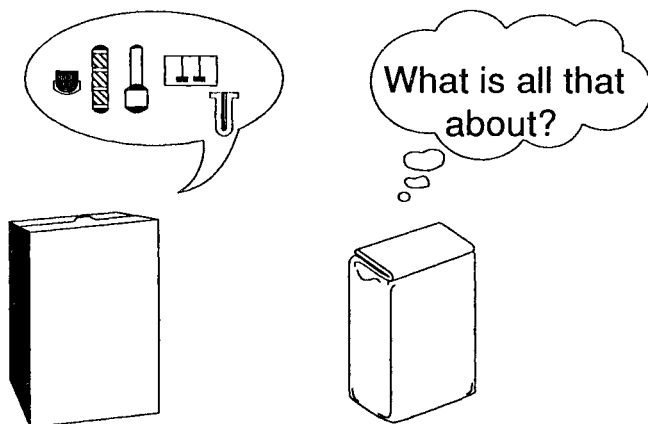


Figure 3: Dialogue Boxes

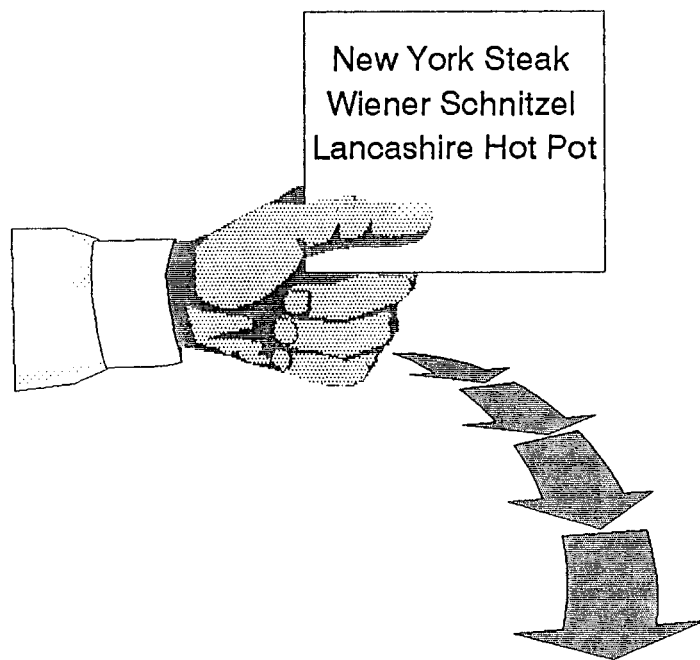


Figure 4: Pull Down Menus

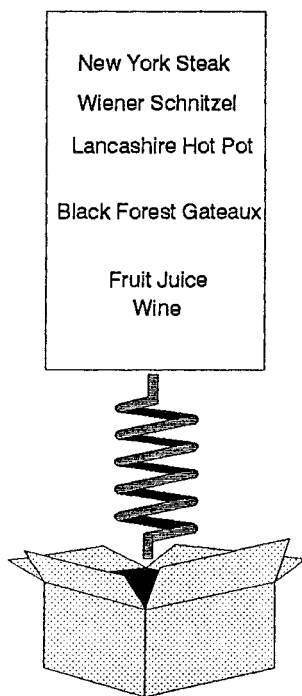


Figure 5: Pop Up Menu

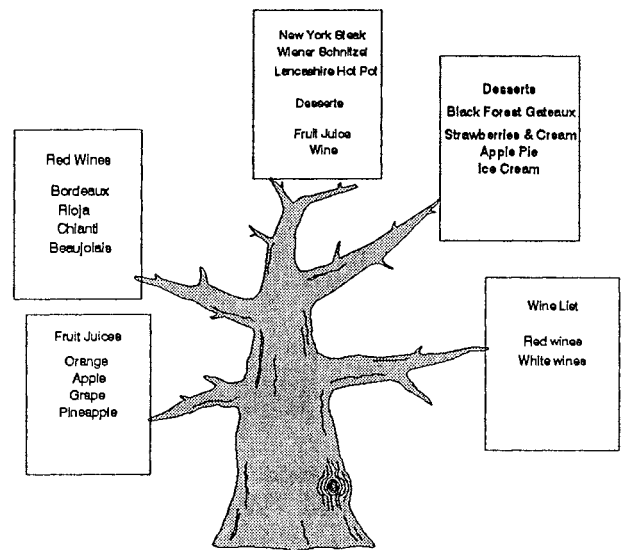


Figure 6: Menu Tree

were and you repeatedly find yourself executing the same set of instructions to get to a location you just left. This is not just a failing of technical programs, the word processor with which I am creating this article suffers from the same problem.

Spreadsheets

The most widely used computer tools are spreadsheets and word processing software. Many engineering software packages now use spreadsheets of a fairly limited kind for data input and the use of spreadsheets in engineering software is likely to become more widely used in the future. I submit that the quality of most existing spreadsheet input forms needs to be improved. Here are some suggestions, all drawn from experience with existing programs as well as our own software.

1. Spreadsheet layout should be simple and uncluttered. They should not require (or even hint at

requiring) the entry of items that are not absolutely necessary.

In our own software we make extensive use of what we call conditional spreadsheets. When the user enters this type of spreadsheet for the first time, asterisks (*) indicate data entry fields that must be filled in by the user. In some cases locating the cursor on an asterisk and pressing <Enter> causes the program to display a list of acceptable options. When the user selects one of them the program returns to the spreadsheet where additional asterisks will indicate data fields that must be filled in. The particular fields that are open to the user will depend on the choices made on the options field. If the user later changes their mind, the old choices will be discarded and new decisions will have to be made.

2. Movement around the spreadsheet should be with the acceptable cursor movement keys (<Up>, <Down>, <Left>, <Right>, etc.). A spreadsheet field to the left of another should be reached using the <Left> key, not with the <Down> key or the <Return> key or anything else nonstandard (and yes, there is at least one package where this rule is not followed as closely as it should be).

3. Data entry fields must be editable. I don't want to have to retype completely a lengthy number or character string in order to correct an error I made entering it yesterday.

4. Typing anything (or pressing <Enter>) while the cursor is located on a data entry field should cause the program to enter data entry mode where the edit keys function (home, end, left, right, Control backspace etc). Once in edit mode, <Escape> should clear the edit mode, not the current entry screen. Pressing <Escape>

in edit mode should restore the last entry.

There is (at least) one commercial software system where — not only are the data entry fields not editable — pressing <Escape> (in a vain attempt not to change the string you started to retype) takes you out of data entry mode AND removes the entire spreadsheet from the screen leaving you with the next spreadsheet in a sequence. What is more, you have to cycle through several other screens, none of which you have the slightest interest in displaying, in order to return to the screen from which you were evicted.

5. Spreadsheet fields should, if it is appropriate for them to do so, accept a units label after a numerical entry that is different from the default units set. The program should perform instant unit conversions and display the result in the default unit set. For example, suppose the default units for length are meters, it should be possible to enter a length of 1.5 meters in either of the following forms (the space is optional):

1.5
1.5 m
150 cm
1500 mm
4.9213 ft
59.0551 inches
59.0551 in

and so on. Thus, the result displayed in response to any of the above entries is 1.5 or 1.5 m.

6. Spreadsheet fields should allow formula entry and calculation modes. Suppose I do not know the numerical value of some particular entry but I know how to calculate it, I should be allowed to enter a calculation sequence. For example:
$$4.3 * 2.1 / (12 - 3.456)$$

The program should display the result after <Enter> has been pressed. A second press of <Enter> should enter the value into the spreadsheet.

7. In the same vein, the calculation mode should accept a certain number of predefined character names as variables with some significance. For example:

0.6 * trayd
0.6 trayd
0.6trayd

are evaluated as 60 percent of the tray diameter.

8. In most cases no entry should be signalled in a special way. A zero or any other numerical value is not acceptable as an unset entry. A better symbol is the *. There is one engineering software package that gives incorrect answers when a zero is left as the default response to a particular spreadsheet field and fails completely when a zero is the desired response (even though zero is a valid and often desired entry).

In case you believe that all of this is too much to ask for, let me assure you that you will appreciate these capabilities if you have them. All of the above are available in our software; all of them are used.

Designing for Novices and Experts

The difference between novice and expert users is illustrated by analogy in Figures 7 and 8. The novice user is a passenger on the airliner in Figure 7 (in the first class cabin, of course). The expert is the pilot of the high performance single-seater jet in Figure 8.

Software developers can cater to novice users by providing an autopilot which guides the user step by step through the data entry and problem solution procedure. At its most basic level of

implementation, the autopilot means programming menus with a memory as discussed above and conditional spreadsheets where the completion of one field leads automatically to the next.

The expert needs no guide but is willing (and able) to take any route in order to reach the appropriate destination. In fact, the expert will want to fly through the software in ways that the designer never had in mind. It is, therefore, a good idea to provide a facility for the user to program their own paths.

It is vitally important that software not allow the user to do anything stupid. I know of one graphical user interface to a commercial flowsheeting program that allows the user easily to create physically impossible flowsheets. Unfortunately, it is impossible to undo the action that created the absurdity and it is necessary to redraw the flowsheet from scratch. Experts know how to avoid the traps and pitfalls that you have (unknowingly) built into your software. If your software permits users to do silly things, novices invariably will find the way to do it.

Software should not require the user to enter any more information than is absolutely necessary. In other words, don't ask the user to enter data that is totally irrelevant to the immediate problem. The experienced user learns to disregard the irrelevant entries in the data entry parts of your program but the novice is forever asking what is the appropriate response to a question that should not have been asked in the first place. The use of conditional spreadsheets can help alleviate this problem which plagues many technical software packages.

One way of helping the novice user is to provide a restricted set of choices. Eliminate (or hide) menu (or list) options that may be likely to make the problem harder to solve. Novice users

Design for novices...

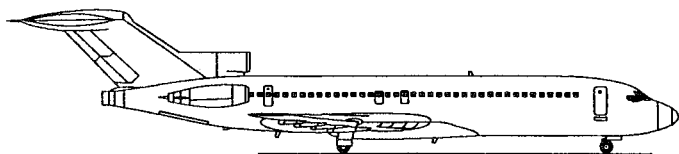


Figure 7: Design for Novices

But allow for experts!

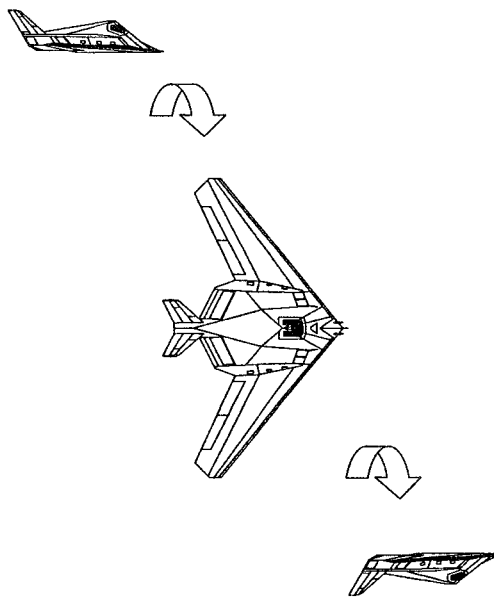


Figure 8: But Allow For Experts!

are sure to pick the options that make the problem harder to solve. Experts will want all possible choices to be available and will accept the responsibility for making sensible choices as well as the consequences of a poor choice.

Technical software should provide a data checking facility that ensures that there are no missing data and no logical inconsistencies. Experts may not need (or want) the data checking facility so it should be possible to turn it off.

Help, I need Somebody!

Novices need lots of help. Experts (by definition, users who think they do not need any help) will not need to use the help system quite so extensively. Software developers know, however, that even experts need help from time to time.

Most sophisticated software these days has context sensitive help messages.

Help should be available at the touch of a key. In many PC based programs help is made available by pressing F1; this is what is meant by simple although it is certainly not "intuitive" (this is supposed to be one of the desirable but elusive attributes of an outstanding software system). The help system should be fully indexed (hypertext) and it should be possible for the user to walk around the help system to find additional information without exiting help mode and moving to some other location in the program before pressing the help key again. Help messages should be clear and provide examples of proper response where appropriate.

Help can also be used to dispense advice to the perplexed. For example, the selection of appropriate thermodynamic models can be difficult in some cases (students especially have difficulty with this). Help can be used to provide recommendations.

Alternatively, a second function key

(F2 say) could be used to provide information of this kind.

I am tempted to include printed documentation under the heading of help. It is the author's opinion that manuals should be written but not read (except as a last resort). When I get a new software package I want to try it immediately. I cannot be bothered reading the manual. If I can't use the package (at an elementary level at least) without reading the manual (with the possible exception of the installation instructions), then the software is deficient. I am pleased with the manual that I wrote for *ChemSep* but I do not know if it pleases our users because no one ever reads it; I like to think that it is because they don't need to.

Based on my experience writing the manual for *ChemSep* I can now say with considerable authority that writing users' guides and the like must rank as one of the worst jobs in the world. I have considerable respect for

those individuals that can write good quality users' guides (a very small fraction of those involved in the very large computer literature business). It is interesting to note that the worst users' guides usually are written by members of the team or company that created the software. For this reason I look forward to the Waite Group's guide to [insert your favorite flowsheeting program name here] and Multicomponent Distillation Made Simple from Microsoft Press.

Coda

There is no doubt that there is much excellent software to be found these days and the limitations are more and more confined to the user interfaces as the engineering challenges are being solved more rapidly than are the user interface design issues. This trend is likely to reverse itself in the future when interface design is of a uniformly high standard. I believe that interfaces to technical software were as bad as they were for so long because users were willing to put up with a lousy interface if the program had the technical capabilities we needed and we could not get them elsewhere. Fortunately, this era has ended.

Acknowledgments

The author would like to acknowledge the major contributions of Harry Kooijman and Arno Haket in the creation of *ChemSep*. Our collaboration on the development of this and other software packages has helped form many of the opinions expressed in this article. Dr. Malcolm Woodman gave the author his first opportunity to speak on some of the topics considered in this article and Peter Rony invited the author to put it in writing. Ron Bondy read an early draft of this article and provided constructive comments and suggestions (some of which appear above). He also encouraged the author

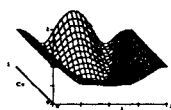
that he is not out in left field (at least not all the time).

Biosketch

Ross Taylor is a professor of chemical engineering at Clarkson University where he has been since 1980. His interests center around mass transfer and process design. He is a coauthor of Multicomponent Mass Transfer to be published by John Wiley and Sons in 1993.

Numerical Methods for Problems with Moving Fronts

by
Bruce A. Finlayson



Dispersion Diagram—see page 546

Highlights

Complete exposition of important methods
Comparison on several test problems
Application of best methods in many fields
• adsorption • reaction • combustion
• melting • oil/water in porous media
• polymer flow • partially saturated flow

See these methods
compared:

Finite Difference
MacCormack
QUICK
Finite Element
Petrov-Galerkin
Taylor-Galerkin
Flux-corrected Methods
TVD & ENO
Random Choice
Moving Elements
Euler-Lagrange

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Communications

Computing and Systems Research at Purdue University

by Joseph Pekny

The School of Chemical Engineering at Purdue University has a strong commitment to pursuing process systems and computing research. Five (Professors Andres, Doyle, Pekny, Reklaitis, and Venkatasubramanian) of our twenty four faculty and twenty seven of our one hundred thirty graduate students conduct research in the traditional systems areas of process control, diagnosis, design, management, monitoring, and simulation. Research is also conducted in enabling technologies including optimization, combinatorics, graph theory, numerical methods, parallel and distributed computing, algorithm engineering, software development techniques, and artificial intelligence methodology.

A heavy concentration of resources in the computing and systems area has a number of advantages. In particular, systems research necessarily involves a cross-disciplinary approach that mixes various aspects of applied mathematics, chemistry, computer science, and physics with engineering principles. Faculty members naturally develop strengths in areas of interest. Close collaboration among the faculty in our research program often catalyzes advances since successful solution of problems often requires expertise in two or more areas. Practically, the collaboration among systems faculty takes the form of jointly advised students, sharing of computer resources, short courses to train graduate students in key technology areas, and a dedicated seminar series involving guests from

industry, computer science, mathematics, and other branches of engineering. From an education point of view, students benefit from exposure to a wide cross-section of ideas and philosophies.

We invest heavily in infrastructure to support systems and computing research by maintaining a current mix of twenty six dedicated IBM, Hewlett Packard, and Sun Microsystem workstations in addition to generally available departmental equipment. This hardware provides faculty and students with access to a number of commercial software packages for process modeling, numerical algorithms, computer-aided software engineering (CASE), thermodynamic properties, and distributed computing.

Our research program also benefits from Purdue's membership in the Multiple-Instruction Multiple-Data (MIMD) Supercomputing Consortium. Purdue maintains a sixteen processor Intel hypercube on campus for algorithm development and access to a five hundred plus processor machine with other consortium members. In addition, we were recently awarded over \$500,000 in hardware from the Hewlett Packard Foundation for the purpose of developing an advanced process systems classroom for undergraduate and graduate education. The twenty two high performance, large memory workstations provided under this grant will allow us great flexibility in incorporating sophisticated computer applications into our curricula. For example, they will permit us to expand the use of computer based laboratory modules pioneered by Professor Squires and several companies that simulate a variety of industrial processes and experiments. In this way, a large number of students can benefit from interaction with industrial technology when direct exposure would be prohibitively expensive, dangerous, or impossible because of physical constraints. The

new classroom will also be available for research use and will make innovative graduate course instruction possible for topics involving extensive graphics, distributed computing experiments, and professional software development tools.

The School of Chemical Engineering has always maintained strong ties to industry as a means for maintaining relevant educational and research goals. Recently, in conjunction with several chemical process industry companies, the Computer Integrated Process operAtions Center (CIPAC) was formed as a vehicle for promoting rapid technology exchange, identifying and investigating process operations problems with industry wide impact, and educating students to develop new theory and methodology to solve real problems. Currently, CIPAC sponsors projects in data reconciliation, qualitative trend analysis, the use of neural networks in monitoring and diagnosis, the development of large scale algorithms for process scheduling, nonlinear modeling for process control, and the construction of tools to reduce the time for developing optimization algorithms. In addition, CIPAC supports faculty/student in-residence programs at member sites as well as an industrial residence program at Purdue. The case studies that result from these interactions prove and validate new technology and, in several cases, the resultant prototype software has been directly or indirectly applied to solve problems at industrial research and manufacturing sites.

The next several years promise to be an exciting time for systems and computing research since the underlying technology continues to evolve at a dramatic rate. This evolution spawns enormous opportunities in systems and computing research as lower level hardware and software advances make possible continuing improvements in process efficiency and open new

research avenues. Our program is harnessing this evolution by exploring areas such as the modeling of molecular phenomena and the development of new frameworks for molecular design. An additional three faculty (Professors Caruthers, Talbot, and Wiest) and twelve graduate students within the School of Chemical Engineering conduct research in computational chemistry and in recent years a number of projects have arisen that integrate systems and chemistry research. Given the importance of molecular based research to agricultural, biological, materials, medical, and pharmaceutical applications further integration of systems and chemistry research promises to be a growth area for several years.

One of the determinants of the pace of evolution in computing technology has been improvements in Very Large Scale Integration (VLSI) fabrication processes. Indeed, greater understanding of the complex transport processes underlying the manufacture of computer chips has been one of the keys to improved yields and circuit capability. In conjunction with electrical engineering faculty, Professor Takoudis leads a team of three chemical engineering graduate students in a computational exploration of transport phenomena underlying fabrication processes. The extreme physical conditions, complexity, and the need for mechanistic understanding of these processes necessitate computational investigation. The need to sustain technology advances and economic competitiveness will accelerate computational research in this area.

Mathematical principles are at the center of most computing and systems research projects. As computing technology advances, it supports the application of more sophisticated mathematical methodology. Professor Ramkrishna and six graduate students investigate applied mathematics and

its interface to computing and systems approaches. Current research topics include the study of pattern formation in catalytic reactors, cybernetic ideas to model bacterial cultures in biological processes, inverse problem methodologies for studying droplet phenomena, and transport and chemical reaction in fractal heterogeneous media. When combined with traditional system research techniques, this promises new tools for investigating complex process phenomena. As parallel and distributed computing capability continues to increase, these new tools will become practical for a large array of important systems and computing applications.

Linnhoff March Offers Process Integration Software and Training to Universities and Industry

by H. Dennis Spriggs, Linnhoff March, Inc.

Process integration techniques based on Pinch Technology have evolved steadily over the past 10-15 years. This methodology is now used routinely by engineering and operating companies worldwide to develop improved process designs. It is used in many different situations to address a variety of design problems. Typical results include reduced energy consumption, lower capital expenditure, reduced emissions, and increased throughput.

Linnhoff March is now making this technology available to universities and is increasing its availability to industry. The program consists of three components: training, software, and university instructional modules.

A three day training course in Pinch Technology is now being offered through AIChE. The course is jointly presented by Linnhoff March, the

University of Manchester Institute of Science and Technology (UMIST), and Exxon Chemical. Among the lecturers are Professor Bodo Linnhoff, one of the primary developers of Pinch Technology, Dr. Vikas Dhole, a principal researcher at UMIST, and Dr. W.R.L. Thomas, a leading practitioner and developer of Pinch Technology at Exxon. In 1993, the course will be offered in Atlanta and Seattle during August and in St. Louis in November. AIChE will publish specific details soon.

The second component of the program is university use of SuperTarget™, Linnhoff March's software for applying Pinch Technology. SuperTarget™ is a PC-compatible process design package using the Microsoft Windows™ graphical user interface.

SuperTarget™ has been developed and evolved over the past 10 years. It contains the latest developments in Pinch Technology in a form convenient for practicing engineers. This software is licensed worldwide to industry and is used internally by Linnhoff March engineers.

The third element of the program is instructional modules and consultation in the preparation and delivery of university instruction. Linnhoff March will provide course outlines in the subject matter, fully developed modules prepared by university staff and/or provide guest speakers for seminars from the U.S. based Linnhoff March staff, several of whom have university teaching experience.

The software and instructional modules will enable university students to become aware of the latest process integration technology and to gain initial applications experience. They will enter industry more fully prepared to apply these techniques on the job.

Professors or students interested in obtaining a university license for SuperTarget™ or gaining access to

instructional materials or speakers should contact: Linnhoff March, Att'n: H. D. Spriggs, 107 Loudoun Street, S.E., Leesburg, VA 22075. Phone: (703) 777-1118, Fax: (703) 777-4145. The license to SuperTarget™ and the use of the instructional materials are provided to universities without charge.

Persons wishing to attend a three day course should register through the AIChE. The 1993 offerings will be held in conjunction with the Atlanta Heat Transfer Conference in August, the Summer AIChE meeting in Seattle, and the St. Louis Annual AIChE meeting in November.

Evolution of Technical Computing in DowElanco

by Gary E. Blau, *Global Ag Math Modelling and Analysis* and Kay E. Kuenker, *Research Information and Statistical Services*; DowElanco, Indianapolis, IN

Introduction

Given the current economic climate, many of the larger industrial companies are taking identifiable business units, usually specialty divisions, and developing them into separate autonomous businesses. In order to achieve a significant market share, these new businesses are frequently formed by the merger of similar business units from different companies into a subsidiary of one or a joint venture of both parent companies. This article describes the evolution of a technical computing function in a new company following the merger of the agricultural chemical divisions from two separate companies. The technical computing function was created in response to a specific direction set by management at the outset of this joint venture. It is hoped that the experiences presented here can be of

value to others involved in similar situations.

DowElanco was formed as a joint venture in 1989 by combining the agricultural chemical divisions of Dow Chemical and Eli Lilly and Company. DowElanco, with sales of 1.5 billion dollars and 3,050 employees worldwide, is headquartered in Indianapolis, Indiana. Having completed a new R&D Center, construction continues on an administration building which will be occupied in 1994. One interesting aspect of this new venture is the role of the parent companies in process research and manufacturing. The manufacturing facilities are owned by DowElanco but are located mostly on Dow or Lilly sites. Operations and process research support are provided by the parents under contract to DowElanco. This relationship has necessitated close interactions with both parents and provide a forum for synergistic development of technical resources to solve DowElanco problems.

Technical Computing Needs

Soon after the announcement of the joint venture, the R&D director and his staff met to develop the guiding principles for DowElanco Research and Development. One of the tenants from this document reads as follows:

"We believe that to be competitive it is essential that we incorporate QUANTITATIVE THINKING and modelling in every aspect of the research and development process from (new product) discovery to ultimate commercialization."

Among the technical computing expertise required to facilitate such quantitative thinking and decision making in an agricultural and specialty chemical company are the following:

- **computational chemistry/chemometrics** – the use of computers to simulate the charge distribution of molecules to help define the mode of action and guide discovery chemistry synthesis programs.
- **statistical analysis** – the design and analysis of field experiments to efficiently determine the efficacy and selectivity of new products.
- **mathematical modelling** – characterization of the behavior of products in the field to better understand their performance.
- **process optimization** – determination of the operating conditions required to minimize the manufacturing costs and by-product formation from existing manufacturing plants.
- **combinametric optimization** – optimal design and scheduling of multiproduct batch plants.
- **operations research** – the optimization of various discrete decision-making processes such as scheduling, project planning, and project prioritization.

Software Selection

In developing an effective technical computing function, software selection was one of the first issues that needed to be addressed. With the exception of combinametric optimization, various software packages were being used by researchers in the parent companies to perform the different tasks on the above list. When the different groups of scientists were using the same software package, e.g., the Simusolv* computer program for dynamic simulation and model building, the decision was obvious. However, when different packages were being used to perform similar tasks, e.g., SAS** and RS/1***, the selection process became more difficult. Scientists had their favorite packages and code conversions would be necessary if only one package were selected. Ultimately, economics

and software support considerations prevailed over individual prejudice in driving the decision.

Platform Selection

Similar to the phenomena that scientists had their favorite computational software, the same held true for computer platforms, both desktop machines and mini/mainframes. When DowElanco was formed a technical architecture decision had not been made. The mode of operation tended toward crisis management and little thought was given as to whether or not a computer equipment purchase coincided with a long term strategy. The only computer platform standard that was enforced was that purchase of desktop machines be limited to either Mac or DOS. Given this option, the vast majority of U.S. based R&D has moved to the Apple Macintosh platform for general desktop computing. Primary reasons for this are that the Macintosh is easy to use, has inherent graphics capabilities which allow scientists to easily draw structures, and requires minimal startup time when beginning on a new machine.

On the mini/mainframe end of things were a group of VAX's**** and one mainframe. R&D was the major consumer of the VAXs while the mainframe was primarily used for commercial and financial applications. The VAX's were soon saturated as the scientists from the parent companies began to use consolidated applications software installed on these machines. As a result, those scientists engaged in technical computing were forced to migrate from performing computations on the VAX to desktop workstations. In addition to the capacity constraints, the lower cost of software for workstations versus mini or mainframes, and the personal control of the machine itself made this decision easier. These workstations, primarily UNIX, are the main source of computing horsepower for the technical

computing groups. The VAX's are used mainly as a source of connectivity to the parent companies and locations from which DowElanco utilizes supercomputers as well as for data storage and data base systems.

All Macintosh and PC computers are connected via ethernet to a corporate-wide LAN at the Indianapolis site. The operating system chosen for this allows UNIX, DOS, and Macintosh computers to communicate for printer, data and application sharing.

Group Formation

Another major issue that needed to be addressed was determining the size and composition of the technical computing group. If the group were too small, then the individuals would feel isolated with little peer interaction and technical back-up is nonexistent. The other danger was to allow the group to become too large because of the number of applications encountered during the company's startup. At DowElanco we had a large number of startup opportunities. Existing chemical plants needed immediate attention to reduce operating costs and minimize unwanted by-product streams. The field experimentation program needed to be integrated on a global basis with experimental farms from both parent companies. It was necessary to merge two different new product development programs into a single program with an optimal distribution of resources across several functions. A radical shift in manufacturing philosophy was required to accommodate the many new products scheduled to come out of the new product development pipeline.

A final issue that needed resolution before an effective technical computing function could be formed was a means for evaluating the performance of the individuals in the group and relating this performance to other scientists more in the mainstream of R&D. A professional career progression

program was established to resolve this issue. In addition, a formal performance management program was introduced that requires each scientist to work with his supervisor to formulate annual expected results. This exercise provided management with realistic expectations for meeting both short- and long-term technical computing needs and served as the vehicle for determining the size of the technical computing group in R&D.

Areas of Excellence

Because of the unique relationship with the parent companies, there are many opportunities for synergism in the technical computing areas. However, with the foundational emphasis on quantitative decision making in DowElanco, it has been necessary to develop in-house expertise in the following areas:

Process Optimization: Dow Chemical is a world leader in continuous processing technology. However, most of DowElanco's products are produced using batch processes. These processes are low volume, exhibit complex chemistry, have high purity requirements, and involve many phases. This difference has stimulated the need to develop in-house math modelling expertise for the design and optimization of batch processes. For example, a study was initiated to maximize the yield and minimize the impurities from a highly exothermic batch process. A kinetic model was built using the Simusolv* computer program from data generated in Dow's laboratories. Then the maximum principle was implemented using Simusolv to determine the optimal batch temperature profile for any production level (Keeler et al., 1992).

A major tenant of the vision of DowElanco is to produce one new product per year. These new products are highly efficacious, requiring only a few grams of active material per acre. Consequently, the annual production

levels are low, but given the complex chemistry, the number of unit operations is high. The design and scheduling of plants to produce these molecules is further complicated by uncertainties in the demand forecasts resulting from market pressures and variable pest infestation levels. A joint research project has been initiated with Professors Reklaitis and Pekny in the chemical engineering department at Purdue University to develop a methodology for batch plant design under uncertainty. Currently, the problem has been formulated as a structured nonlinear integer program. Close collaboration with the principle investigators will be required to insure that the resultant combinatorial algorithms developed will be adequate for handling problems of the magnitude and degree of uncertainty encountered in DowElanco. The challenge of the technical computing group will be to take these developments and apply them to the chemistry and process engineering inherent in our specific products.

Probabilistic Network Modelling:

Given DowElanco's commitment to launching a new product every year, it is essential that the new product development pipeline be efficient. Every year, over 30,000 new molecules are screened for activity and selectivity as herbicides, fungicides, and/or insecticides. From these molecules, a few candidates are selected to enter the new product pipeline. While in the pipeline each candidate undergoes a large number of tests designed to determine efficacy and potential environmental and toxicological impact. The result is that only those molecules with the highest economic potential and negligible environmental impact are submitted for registration to government agencies. The cost of this process is formidable, involving scientists from many disciplines such as process research, formulations, environmental chemistry, biology, toxicology, and entomology, etc. Field research studies

are conducted on a global basis to validate product concepts and ensure performance under a variety of crop and climatic scenarios.

A probabilistic network model was built to simulate the behavior of this new product development process. Because of the discrete nature of this process, SLAM System*, (Pritsker, 1986) was chosen as the simulation language instead of Simusolv. A probabilistic description of the time and resources required for each task performed was captured in the model. This was a complicated exercise requiring interaction between many functions. The very exercise of building the model turned out to be an excellent vehicle for fostering communication between the functions as well as generating a preferred sequence of activities for the development process. The model serves as a pilot plant for individual scientists and management to answer "what if" questions. It is also being used by management to perform optimal resource allocation studies to achieve the vision of one new product per year.

Probability Modelling for Risk

Assessment: By their very nature agrochemical products are introduced into the environment. One of the greatest challenges facing producers is to ensure that the risk of harmful exposure to humans and non-target organisms is minimal. Existing compounds which are highly soluble, volatile, or extremely persistent have already been removed from the marketplace. New products exhibiting these characteristics are eliminated in the screening process mentioned earlier. Although the new families of agrochemicals are highly active to the pests they are designed to control, they are more benign to the environment. It is important, however, to develop tools for assessing the risk associated with these products to alleviate any public

anxiety in using agricultural and specialty chemicals.

Several deterministic models have been built to characterize the fate of chemicals in the environment. They predict sequential concentration-time data in the air, in water runoff, or in the soil following chemical application for a given climate scenario. Air dispersion models are based on a Gaussian plume assumption and are extremely sensitive to local meteorological conditions such as wind and air stability (Blau et al., 1992). Models of chemical transport in the soil consist of a hydrological balance, a heat balance, and a chemical reaction/dissipation component. These systems of partial differential equations in position and time must be solved for a set of stochastic boundary conditions which represent rainfall, temperature, radiation, and any other significant climatic parameters. An additional challenge in using these models is the heterogeneity of the soil matrix. Soil types vary with depth from field to field and even within fields. As a result, the solution of the deterministic model systems are valid for only one climate scenario and specific soil type. In order to generate meaningful results, the stochastic nature of the climate and the uncertainties inherent in the soil matrix must be reflected in predictions made with the model. In other words, the output from these models must be concentration probability distributions at specified times and distance from the source of application. These probability distributions can then be combined with toxicological end points to perform meaningful risk assessments. An even simpler use is to estimate the probability of significant runoff or movement into ground water at a specific location.

The determination of the probability distribution for the climate and soil matrix is a major challenge. For the former, an approach developed by Richardson has been used (Richardson

et al., 1984). Here the probability of rainfall at a specific location is characterized by a simple Markov process. Then the magnitude of the rainfall is shown to follow a Gamma distribution. The temperature and radiation are characterized by the parameters of a Fourier series conditional on the wet or dry status of a day. Meteorological data available from various weather stations are used to estimate the parameters of the climate model and then interpolated to specific field locations. Extensive data base manipulations are necessary to determine the distribution for soil parameters such as percent organic matter, permeability, etc., as functions of depth and location. Although this information is supplied by government agencies, it is a nontrivial task to produce the distributions in a form compatible with the soil/climate models.

Once the probability distributions for all the climatic and soil parameters are specified, a Monte Carlo sampling strategy is used to select scenarios from these distributions. The number of parameters is so large (i.e., greater than 30) that the number of Monte Carlo runs required to produce meaningful results is impractical. As a result a sensitivity analysis is conducted on the set of parameters and a smaller subset of parameters is selected. A comparison has been performed (Fontaine et al., 1992) between a simple linear sensitivity analysis and a core complex but global Fourier Amplitude Sensitivity Test (McRae et al., 1984) for a specific climate-soil model in the U.S. corn belt. In this application the linear analysis produced the same list of prioritized parameters as the FAST method.

Since the computational structure of the Monte Carlo runs are "embarrassingly parallel," these calculations can be performed on parallel computers. This result is particularly important because performing risk assessments on

responses in the vicinity of 1 in a million require a large number of Monte Carlo runs to adequately characterize the tails of the distributions. For example, to estimate the probability of a significant runoff following a 100 year rainfall event shortly after application at a specific location may require well over 10,000 Monte Carlo runs. Determining the optimum number of trials and how best to utilize the evolving parallel computing resources are ongoing research projects.

Conclusions

Participating in the formation of the technical computing function for DowElanco has been a stimulating exercise. In the next few years the value returned to this joint venture through the emphasis on quantitative thinking and modelling will be reflected in the marketplace.

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- * Simusolv a trademark of Dow Chemical Company
 - ** SAS a trademark of the SAS Institute
 - *** RS/1 a trademark of BBN Company
 - **** VAX trademark of Digital Equipment Corporation
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Meetings, Conferences, Congresses, Short Courses, and Workshops

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

1993 AIChE Spring National Meeting

Houston, TX
March 28–April 1, 1993

The CAST Division is sponsoring the following sessions at the Houston National meeting.

Area 10a: Systems and Process Design

1. New Advances in Process Synthesis and Analysis (Ciric/El-Halwagi)
2. Industrial Applications of CAD (Motard/Britt)

Joint Area 10a and Area 11 Session

1. Design for Safety and Environmental Impact (Ciric/Tarantino)

Joint Area 10a and Area 15 Session

1. Bioprocess Design and Simulation (Chan/Stramando)

Area 10b: Systems and Process Control

1. Industrial Applications in Process Control (Mijares/Bailey)
2. Nonlinear and/or Predictive Control in Practice (Hawkins)

Area 10c: Computers in Operations and Information Processing

1. Expectations from Plant Process Integration Techniques [Panel Discussion] (Robertson/Zilora)
2. Process Modeling and Optimization (Wellons/Tjoa)
3. Integration in Planning and Operations (Bodington, Coon)
4. Electronic Process Data Exchange – The PDXI Project (Baldwin, Myers)

Modeling and Optimization in Process Design and Operation

Engineering Design Research Center, Carnegie Mellon University, Pittsburgh, PA
May 23–28, 1993

This is a reorganized 6-day course that stresses model formulation and solution in the areas of process design and operation. Attendees will learn to create and solve such models more systematically, obtaining from the course the necessary background to understand the modern tools which are now available and to apply them effectively and efficiently. It is aimed at modeling practitioners and technical managers who do not wish to treat process modeling as a black art.

Topics of this course include concepts for process model formulation (object oriented modeling, getting degrees of

freedom right, discovering why a model will not solve), strategies for flowsheet optimization, concepts for process synthesis (heat integration, [nonideal] separation systems, reactor networks), mixed-integer optimization models for synthesis, optimization of differential/algebraic systems, and planning and scheduling of batch processes.

Course participants will address these topics through lectures and hands-on workshops, making extensive use of the ASCEND and GAMS computer software. Course participants will receive a comprehensive set of lecture notes and the CACHE Collection of Optimization Case Studies along with the GAMS software for running on IBM PC compatibles.

The instructors of the course are Professors Larry Biegler, Ignacio Grossmann, and Arthur Westerberg. For information please call (412) 268-3372 (e-mail: TM2L@andrew.cmu.edu), or write to Engineering Design Research Center, Carnegie Mellon University, Pittsburgh, PA 15213-3890, Att'n: Toni McIltrout.

1993 American Control Conference

San Francisco, CA
June 2-4, 1993

The 1993 ACC will be held in San Francisco on June 2-4, at the Westin St. Francis Hotel.

Conference Highlights

The 1993 American Control Conference has 14 parallel sessions each day on topics spanning current developments in the applications and theory of control systems engineering. The program includes 528 contributed papers and 220 papers in 33 invited sessions on special topics. A special "video" session has been organized

highlighting current experimental control research. The videotape presentations from this session have been compiled onto a single tape which will be available to purchase at the conference.

There will be three plenary sessions: Dr. John Cassidy, Vice President, United Technologies Corporation, will speak on "Control Technology and the 21st Century;" Professor Stephen Boyd of Stanford University, winner of the 1992 Eckman Award, will speak on "Control Systems Analysis and Synthesis via Linear Matrix Inequalities;" and Professor Sanjoy Mitter, director of the Laboratory for Information and Decision Systems at MIT, will present current research in intelligent control in his talk entitled "Perception, Cognition, and Situated Actions."

Pre-Conference Workshops

Seven tutorial workshops (short courses) have been organized for the two days prior to the ACC, May 31 and June 1.

Two Day Workshops – May 31 and June 1:

1. Intelligent Control
2. Behavior Design and Analysis using State-charts
3. Numerical Methods for Control System Design (with Emphasis on State-Space Models)
4. Real-Time Applications in Control Using Digital Signal Processors

One Day Workshops – June 1:

5. Automated System Identification and Control with Applications
6. Nonlinear and Adaptive Control
7. Petri Net Modeling, Control and Performance Analysis for Manufacturing Systems

The workshop lecturers are leaders in their fields who have published

extensively and are experienced lecturers.

For more information, contact Abraham H. Haddad, General Chair, Department of EECS, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3118; (708) 491-3641; ahaddad@eecs.nwu.edu.

1993 ASEE Annual Conference

**Urbana, IL
June 20-24, 1993**

At the 1993 Annual Conference of the American Society for Engineering Education, to be held at the University of Illinois, Urbana, June 20-24, 1993, the Chemical Engineering Division of the ASEE will be sponsoring a program with the theme, "Emerging Areas of Teaching and Research in Chemical Engineering."

The program includes a session on High Performance Computing in Chemical Engineering (Moderator: Mark Stadtherr, University of Illinois), which will focus on opportunities for research and teaching in this area. Other sessions include New Chemical Engineering Research Areas (Moderator: Thomas Marrero, University of Missouri-Columbia) and New Partnerships with Industry in Chemical Engineering Research (Moderator: Neil Book, University of Missouri-Rolla). Since this is the 100th Anniversary of the ASEE, there will also be three sessions emphasizing the history of chemical engineering education.

Information about the Conference can be obtained from American Society for Engineering Education, Suite 200, 11 DuPont Circle, Washington, DC, 20036. Telephone: (202) 986-8500.

AIENG 93 Applications of Artificial Intelligence in Engineering

**Toulouse, France
June 29-July 1, 1993**

The Eighth International Conference on Artificial Intelligence in Engineering will be held from June 29 through July 1, 1993 at the ATRIA Mercure Hotel, Toulouse, France. The purpose of the conference is to provide an international forum for the presentation of work on the state-of-the-art in the application of artificial intelligence to engineering problems. It also aims to encourage and enhance the development of this most important area of research. The previous seven international conferences have stimulated significant presentations on the application of AI in Engineering as well as the tools and techniques required for the successful use of AI in Engineering, as well as many new applications. Conference themes include:

Basic Research in AI – Knowledge representation, validation/verification, constraint propagation, qualitative modeling, model-based reasoning, case-based reasoning, temporal reasoning, fuzzy logic, real-time aspects, neural networks, genetic algorithms, etc.

AI Research Applied to Engineering – Autonomous vehicles, robotics, planning and scheduling, process control, surveillance systems, fault diagnosis, reliability, design, man/machine communication, etc.

Application Domains – Aeronautics and space, manufacturing, energy, transportation, electronics industry, automobile, biomedical engineering, agriculture, chemical engineering, etc.

For more information, contact the conference chair, R. A. Adey, Wessex Institute of Technology, Ashurst Lodge, Ashurst, Southampton SO4 2AA, UNITED KINGDOM.

ESCAPE-3

Graz, Austria

July 4-7, 1993

ESCAPE-3 is a continuation of a series of events initiated by the European Federation of Chemical Engineering Working Party on Computer Aided Process Engineering. ESCAPE-3 will take place at the Conference Center of the International Trade Fair in Graz, Austria. The subjects covered at this symposium will focus on recent developments of computer applications in process engineering in general and in particular on process synthesis, design, and optimization; process dynamics, control, and operation; operation of plants; management, economic, and integration issues; computer aided design for cleaner production; and computer aided bioprocess technology. For further information, contact the Organization Secretariat, ESCAPE-3, Institute of Chemical Engineering, Graz University of Technology, Inffeldgasse 25, A-8010 Graz, AUSTRIA, 43-316-873-7461, 43-316-873-7469 (Fax).

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

Mount Crested Butte, CO
July 18-23, 1993

Cosponsored by CAST Division and
CACHE Corporation.

The second Foundations of Computer-Aided Process Operations conference is scheduled for summer 1993. In contrast to process design and process control, this conference focuses on the need to establish a new discipline of process operations within chemical engineering. The objectives of the conference include an overview of the state of the art in process operations theory and practice, in depth discussion of practical challenges in this field, a better understanding of

new tools available from the research community, and stimulation to focus research on perceived needs and challenges from the process industries. Proposals are encouraged for the poster session, challenge problems, or software demonstrations.

The technical session and presentation titles include:

1. Keynote

"Non Steady States - A New Management Paradigm"

2. Process Monitoring Acquisition, Organization, Storage, and Retrieval for Real Time Applications

"Data Treatment and Applications"

"Model Based Monitoring"

3. Quality Management

"Design and Control for Quality Improvement in Process Operations"

"Total Quality Management"

4. Safety and Environment

"Living with Human Errors in Computer Controlled Plants"

"Incorporating Environmental Objectives in Process Design and Operation"

5. Facilities and Practices to Ensure Product Availability

"Total Productive Management in the Refinery of the 21st Century"

"Managing Reliability and Maintenance in the Process Industry"

6. Flexibility and Integration

"Outlook for CIM in the Japanese Process Industry"

"Integration of Designs, Scheduling, and Control"

"Integration of Monitoring, Diagnosis, and Unit Control"

7. Scheduling

"An Integrated Approach to Planning and Scheduling"

"A General Framework for Optimal Process Planning and Scheduling"

"Learning to Solve Scheduling Problems - The Role of Rigorous Knowledge Acquisition Framework"

8. Plant Wide Management and Control

"Case Study Presentations"

9. Making It Work - Examples of Profitable Applications

"Achieving the Optimum of a Multiplant Chemical Plant"

"A Modular System for Scheduling Chemical Plant Production"

"A Probability Modeling Methodology for Improving Process Operations"

For more information, contact David W. T. Rippin (Conference Chair), Chemical Engineering Department, Swiss Federal Institute of Technology, ETH Zentrum, CH-8092 Zurich, SWITZERLAND, 01-256-3112, 01-252-0975 (Fax), rippin@tcl.ethz.ch or John C. Hale (Conference Vice Chair), E. I. du Pont de Nemours and Company, PO Box 6090, Newark, DE 19714-6090, 302-366-3041, 302-366-4889 (Fax). To apply for attendance at FOCAPO, contact the CACHE Corporation, PO Box 7939, Austin, TX 78713-7939, 512-471-4933, 512-295-4498 (Fax), cache@utxvm.cc.utexas.edu.

IFAC World Congress

Sydney, Australia

July 19-23, 1993

The 1993 IFAC World Congress will include a Mini-Symposium on Chemical Process Control. This Mini-Symposium will be coordinated by the IFAC Working Group on Chemical Process Control and it will emphasize themes from the Contemplative Stance of the Working Group. These themes are: soft sensing, process modeling, model identification, process control algorithms, integration of design and control, safety and environment, and integrated process management. There will be 48 papers in the Mini-Symposium. The deadline for submission of papers was July 31, 1992. However, additional information may be obtained from the IFAC Congress Technical Secretariat, Department of Electrical and Computer Engineering, University of Newcastle, Callaghan, New South Wales 2308, AUSTRALIA or from Tom McAvoy, Department of Chemical Engineering, University of Maryland, College Park, MD 20742-2111, 301-405-1939, mcavoy@eng.umd.edu.

1993 AIChE Annual Meeting

St. Louis, MO

November 7-12, 1993

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

The CAST Division is planning the following sessions at the St. Louis Annual Meeting which have been approved by the Meeting Program Chair. Deadlines and a final call for papers for this meeting appear later in this issue.

Area 10a: Systems and Process Design

1. Design Under Uncertainty.

Sandro Macchietto, Imperial College (Chair) and Stratos Pistikopoulos, Imperial College (Co-Chair).

2. Design and Analysis.

Michael L. Mavrouniotis, University of Maryland (Chair) and Iftekhar A. Karimi, E. I. du Pont de Nemours & Company (Co-Chair).

3. Process Synthesis.

Michael F. Malone, University of Massachusetts (Chair) and Vivek Julka, Union Carbide Corporation (Co-Chair).

Joint Area 10a and Area 10d Session

1. Computational Approaches in Systems Engineering.

Christodoulos A. Floudas, Princeton University (Chair) and Joseph F. Pekny, Purdue University (Co-Chair).

Joint Area 10a and Area 2 Session

1. Synthesis of Complex Separation Systems.

Vivek Julka, Union Carbide Corporation (Chair).

Area 10b: Systems and Process Control

1. Advances in Process Control.

Babu Joseph, Washington University (Chair) and Sigurd Skogestad, NTH (Co-Chair).

2. Identification and Adaptive Control.

Irven H. Rinard, City College of CUNY (Chair) and Thomas B. Co, Michigan Technological University (Co-Chair).

3. Nonlinear Process Control.

Daniel E. Rivera, Arizona State University (Chair) and Francis J. Doyle, Purdue University (Co-Chair).

4. Model Predictive and Robust Control.

Vasilios I. Manousiouthakis,

University of California Los Angeles (Chair) and Oscar D. Crisalle, University of Florida (Co-Chair).

5. Solutions to the Industrial Challenge Problems in Process Control.

Randy C. McFarlane, Amoco (Chair) and James J. Downs, Eastman Chemical Company (Co-Chair).

Joint Area 10b and Area 10c Poster Session

1. Issues in Process Modeling, Optimization, Monitoring, and Control.

Yaman Arkun, Georgia Institute of Technology (Chair), Jay H. Lee, Auburn University (Co-Chair), Spyros A. Svoronos, University of Florida (Co-Chair), and James F. Davis, Ohio State University (Co-Chair).

Area 10c: Computers in Operations and Information Processing

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

(Cosponsored by the International Cooperation Committee of the Society of Chemical Engineers, Japan) Iori Hashimoto, Kyoto University (Chair) and G. V. Reklaitis, Purdue University (Co-Chair).

2. Plant Wide Dynamic Simulation.

Jorge A. Mandler, Air Products and Chemicals (Chair) and Anthony Skjellum, Mississippi State University (Co-Chair).

3. Artificial Intelligence in Process Engineering.

Venkat Venkatasubramanian, Purdue University (Chair) and Mark A. Kramer, Massachusetts Institute of Technology (Co-Chair).

4. Visualization in Chemical Engineering Systems.

Sangtae Kim, University of Wisconsin (Chair) and Alan B. Coon, Union Carbide Corporation (Co-Chair).

Joint Area 10c and Area 10d Session

1. Parallel Numerical Methods and Applications. Anthony Skjellum, Mississippi State University (Chair) and Joseph F. Pekny, Purdue University (Co-Chair).

Area 10d: Applied Mathematics and Numerical Analysis

1. Pattern Formation and Dynamics. Hsueh-Chia Chang, University of Notre Dame (Chair) and Yannis G. Kevrekidis, Princeton University (Co-Chair).

2. Instabilities, Time Series, and Chaos. Julio Ottino, Northwestern University (Chair) and B. Erik Ydstie, Carnegie Mellon University (Co-Chair).

3. Self-Similarity, Scaling, and Renormalization in Chemical Engineering. D. Ramkrishna, Purdue University (Chair) and Fernando J. Muzzio, Rutgers University (Co-Chair).

4. Probabilistic Models. Kyriacos Zygourakis, Rice University (Chair) and D. Ramkrishna, Purdue University (Co-Chair).

In addition to symposia sessions, CAST will also cosponsor with Area 4 (Education) the third annual Educational Computer Software Demonstrations organized by Douglas Cooper, University of Connecticut, and David Greenberg, University of Cincinnati.

1994 AIChE Spring National Meeting

**Atlanta, GA
April 17-21, 1994**

Meeting Program Chair: Soni O. Oyekan, E. I. du Pont de Nemours &

Company, PO Box 1089, Orange, TX 77631-1089, 409-886-9202, 409-886-6264 (Fax).

The CAST Division is planning the following tentative program at the Atlanta National Meeting. AIChE and the Meeting Program Chair will finalize the sessions at the 1993 Programming Retreat in February, and any corrections will appear in the next issue of CAST Communications. Tentative deadlines and a first call for papers for this meeting appear later in this issue.

Area 10a: Systems and Process Design

1. Computer-Aided Applications for the Pulp and Paper Industry. Mahmoud El-Halwagi, Auburn University (Chair) and Harry Cullinan, Auburn University (Co-Chair).

2. Process Synthesis. Luke E. K. Achenie, University of Connecticut (Chair) and Stratos Pistikopoulos, Imperial College (Co-Chair).

3-4. Design and Analysis I and II. Michael F. Malone, University of Massachusetts (Chair) and Jeffrey J. Sirola, Eastman Chemical Company (Co-Chair).

5. Design of Batch Processes. Iftekhar A. Karimi, E. I. du Pont de Nemours & Company (Co-Chair) and Joseph F. Pekny, Purdue University (Co-Chair).

6. Innovations in Process Modeling and Simulation. Robert S. Butner, Pacific NW Laboratory (Chair) and Rakesh Govind, University of Cincinnati (Co-Chair).

Area 10b: Systems and Process Control

1. Model Predictive Control. Yaman Arkun, Georgia Institute of Technology (Chair) and F. Joseph

Schork, Georgia Institute of Technology (Co-Chair).

2. Modeling, Monitoring, and Control in the Pulp and Paper Industries. Ferhan Kayihan, Weyerhaeuser (Chair) and Robert R. Horton, Institute of Paper Science and Technology (Co-Chair).

3. Statistical Process Control. Charles F. Moore, University of Tennessee (Chair).

4. Empirical Process Modeling for Control. Thomas J. Harris, Queen's University (Chair) and Derrick K. Rollins, Iowa State University (Co-Chair).

5. Novel Applications in Process Control. Gerardo Mijares, M. W. Kellogg Company (Chair) and Jonathan E. Withlow, Florida Institute of Technology (Co-Chair).

Area 10c: Computers in Operations and Information Processing

1. Environmental Considerations for Process Simulation and Operations. Stephen E. Zitney, Cray Research, Inc. (Chair) and Urmila Diwekar, Carnegie Mellon University (Co-Chair).

2. Advances in Process Operations: Industrial Success Stories. Mark A. Kramer, Massachusetts Institute of Technology (Chair).

3. Techniques and Practice of Planning and Scheduling in Process Plants. Michael T. Tayyabkhan, Tayyabkhan Consultants Inc. (Chair).

4. Data Analysis for Process Applications. Alan B. Coon, Union Carbide Corporation (Chair) and Rob Whiteley, Oklahoma State University (Co-Chair).

5. Enabling Technologies for Next Generation Process Simulators.

Anthony Skjellum, Mississippi State University (Chair) and Stephen E. Zitney, Cray Research, Inc. (Co-Chair).

6. Application of High Performance Computing in Chemical Process Engineering.

Mark A. Stadtherr, University of Illinois (Co-Chair) and Anthony Skjellum, Mississippi State University (Co-Chair).

Area 10d: Applied Mathematics and Numerical Analysis

1. Numerical Methods for ODE/DAE/PDES. Anthony Skjellum, Mississippi State University (Co-Chair) and Alan B. Coon, Union Carbide Corporation (Co-Chair).

Fifth International Symposium on Process Systems Engineering (PSE '94)

**Kyongju, Korea
May 30–June 3, 1994**

The International Programming Committee announces the Fifth International Symposium on Process Systems Engineering to be held May 30–June 3, 1994 at Kyongju, Korea. Main themes of the conference will include process modeling simulation and optimization, process synthesis and design, process dynamics and control, AI applications to process engineering, computer integrated manufacturing in the chemical process industries, and new technologies in process systems engineering. Deadline for prospective authors to submit 400-600 word abstracts is June 1, 1993. For further information, contact the Conference Secretariat, Professor En Sup Yoon, Department of Chemical Engineering, Seoul National University, Seoul 151-742, KOREA, 82-

2-887-7232, 82-2-884-0530 (Fax),
pslab@krsnucc1.bitnet.

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

**Snowmass Village, CO
July 10-15, 1994**

Cosponsored by CAST Division and
CACHE Corporation

The fourth International Conference on Foundations of Computer-Aided Process Design is scheduled for summer 1994. For more information, contact Michael F. Doherty (Conference Chair), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-0011, 413-545-2359, 413-545-1647 (FAX), mdoherty@ecs.umass.edu or Lorenz T. Biegler (Conference Vice-Chair), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, 412-268-2232, 412-268-7139 (Fax), dl01lb01@vb.cc.cmu.edu.

1994 AIChE Annual Meeting

**San Francisco, CA
November 13–18, 1994**

Meeting Program Chair: Peter Van Opdorp, UOP, 25 E. Algonquin Road, Des Plaines, IL 60017, 708-391-3588, 708-391-3737 (Fax).

The CAST Division is considering the following programming topics for the San Francisco Annual Meeting. AIChE and the Meeting Program Chair will finalize the sessions at the 1993 Programming Retreat in February, and the approved program will appear in the next issue of CAST Communications.

Design and Analysis

Design with Molecular Information

Process Synthesis

Computer-Aided Design of Batch Processes

Design and Control

High Performance Computing in Computer-Aided Design

Advances in Process Control

Nonlinear Control

Model Predictive Control

Robust Identification

Plant-Wide Control

Parameter and State Estimation

Fault-Tolerant Control

Recent Developments in Modeling, Optimization, Computation, Monitoring, and Control

Statistics and Quality Control

Computational and Structural Issues in Nonlinear System

Identification

Advances in Optimization

Process Operations

Data Interpretation

Intelligent Manufacturing Systems

Applications of Chaos and Fractals

Computational Integral and Spectral Methods

Advances in Computational and Applied Mathematics

Techniques for Nonlinear PDEs

Stochastic Systems

In addition, CAST plans to again cosponsor Educational Computer Software demonstrations throughout the Annual Meeting.

FROM ACADEMIC PRESS

Artificial Intelligence in Chemical Engineering

Thomas E. Quantrille and Y.A. Liu

"At long last, here is a comprehensive, yet very readable, exposition of the emerging science of artificial intelligence (AI) as it relates to the practice of chemical engineering...this book is a must read for any serious student of AI in the chemical process industries. In essence, the book covers everything a reader should know about AI, but has long been afraid to ask....This book belongs to a class by itself in providing a thorough coverage of the fundamentals of AI, and illustrating their applications with concrete examples from the CPI. Above all, it is a pleasure to read, unlike, alas, most other books on this fascinating subject."

—CHEMICAL ENGINEERING

Key Features

- Allows the reader to learn AI quickly using inexpensive personal computers
- Contains a large number of illustrative examples, simple exercises, and complex practice problems and solutions
- Includes a computer diskette for an illustrated case study
- Demonstrates an expert system for separation synthesis (EXSEP)
- Presents a detailed review of published literature on expert systems and neural networks in chemical engineering

1992, 609 pp., \$75.00/ISBN: 0-12-569550-0

Polymers for Electronic and Photonic Applications

C.P. Wong

The most recent advances in the use of polymeric materials by the electronics industry can be found in **Polymers for Electronic and Photonic Applications**. This book provides in-depth coverage of photoresists for microlithography, microelectronic encapsulants and packaging, insulators, dielectrics for multichip packaging along with electronic and photonic applications of polymeric materials, among many other topics. Intended for engineers and scientists who design, process, and manufacture microelectronic components, this book will also prove useful for hybrid and systems packaging managers who want to be informed of the very latest developments in this field.

CONTENTS: Overview of Polymers for Electronic and Photonic Application. The Chemistry of Polymers for Microlithographic Applications. Interconnect Dielectrics. Recent Advances in IC Passivation and Encapsulation: Process Techniques and Materials. Polyimides for Electronic Applications. Polyimides-oxanes: Chemistries and Applications. Applications of Epoxy Resins in Electronics. Advances in Thermoplastics for Electronic Applications. Polymers for Increased Circuit Density in Interconnection Technology. Piezoelectric and Pyroelectric Polymers. Polymers for Nonlinear Optics. Polymers as Third-Order Nonlinear-Optical Materials. Polymers for Integrated Optical Waveguides. Langmuir-Blodgett Manipulation of Electrically Responsive Polymers. Basic Concepts of Polymer Mechanical Behavior. Chapter References. Index.

October 1992, 680 pp., \$99.95/ISBN: 0-12-762540-2

The Numerical Method of Lines

Integration of Partial Differential Equations

W.E. Schiesser

This is the first book on the numerical method of lines, a relatively new method for solving partial differential equations. **The Numerical Method of Lines** is also the first book to accommodate all major classes of partial differential equations. This is essentially an applications book for computer scientists. The author will separately offer a disk of FORTRAN 77 programs with 250 specific applications, ranging from "Shuttle Launch Simulation" to "Temperature Control of a Nuclear Fuel Rod."

CONTENTS: What Is the Numerical Method of Lines? Some Applications of the Numerical Method of Lines. Spatial Differentiation. Initial-Value Integration. Stability of Numerical Method of Lines Approximations. Additional Applications: Multidimensional PDEs and Adaptive Grids. Appendix A: The Laplacian Operator in Various Coordinate Systems. Appendix B: Spatial Differentiation Routines. Appendix C: Library of ODE and ODE/PDE Applications.

1991, 326 pp., \$72.50/ISBN: 0-12-624130-9

Dynamic Modeling of Transport Process Systems

C.A. Silebi and W.E. Schiesser

This book presents a methodology for the development and computer implementation of dynamic models for transport process systems. Rather than developing the general equations of transport phenomena, it develops the equations required specifically for each new example application. These equations are generally of two types: ordinary differential equations (ODEs) and partial differential equations (PDEs) for which time is an independent variable. The computer-based methodology presented is general purpose and can be applied to most applications requiring the numerical integration of initial-value ODEs/PDEs. A set of approximately two hundred applications of ODEs and PDEs developed by the authors are listed in Appendix 8.

1992, 518 pp., \$99.50/ISBN: 0-12-643420-4

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FAX **1-800-336-7377**

Call For Papers

A Word About Manuscripts and Visual Aids

It is AIChE policy that all authors submit a manuscript to AIChE headquarters in advance of the meeting. Although permission is granted to AIChE to make copies of the manuscript, copyright ownership, if any, remains with the author. Copies of presentation manuscripts may be ordered from AIChE for delivery by mail after the meeting. Presumably, manuscript copies may also be obtained directly from the author.

AIChE would prefer complete, full-length manuscripts. However, The Executive Board of the Programming Committee has recently determined that an extended abstract with figures, tables, and references will also satisfy their manuscript requirement.

In addition, the CAST Executive Committee has adopted the policy that all speakers at CAST-sponsored sessions shall provide hard copies of their visual aids to the audience in advance of each presentation. Visual aids which follow AIChE guidelines should be readily legible even if reduced to quarter-size and reproduced double-sided. The CAST Division hopes this service will prove especially useful to our audiences.

Call for Papers Instrument Society of America Chicago, September 20-24, 1993

One or two sessions on "Developments in the Engineering Lab," to be held at ISA '93 Chicago International Conference and Exhibition, September 20-24, 1993 (annual meeting of the Instrument Society of America). Papers are solicited that describe: experimental studies of new applications of control theory, and improvements in process control laboratories.

Please contact the session chairman: A.G. Hill, Dept of Chemical Engineering, University of Southwestern Louisiana, Lafayette, LA 70504-4130, Phone: 318-231-5761, Fax: 318-231-6688, Email: aghill@usl.edu.

Final Call for CAST Sessions 1993 AIChE Annual Meeting St. Louis, MO, November 7-12, 1993

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

Special Note to Authors Submitting Abstracts for Any Annual Meeting Session Sponsored by Area 10b (Systems and Process Control):

Because of the large number of anticipated presentation proposals in the area of process control and the limited symposia space available, all proposals to Area 10b will be received centrally by the Area Chair and then rated by a panel of session chairs for selection and allocation to specific sessions. Because of this centralized selection process, the initial deadline for Area 10b is ONE MONTH EARLIER than for other CAST-sponsored sessions:

March 2, 1993 (For Area 10b - Process Control - Only): Submit an abstract (camera-ready) on a completed original new-version AIChE Proposal-to-Present Form and also an extended abstract of 400-600 words to the AREA CHAIR. It is appropriate to indicate for which session the contribution might best fit.

April 1, 1993 (For All Other CAST Sessions): Submit an abstract (camera-ready) on a completed original new-version AIChE Proposal-to-Present Form to the appropriate SESSION CHAIR and a copy also to the co-chair.

April 27, 1993: Session content is finalized. Authors are informed of selection.

September 7, 1993: Authors submit, if desired, any revision to the abstract (camera-ready) to AIChE.

September 24, 1993: Authors submit final manuscript to AIChE.

November 7, 1993: Speakers bring hard copies of visual aids to be distributed to the audience at the presentation.

Area 10a: Systems and Process Design

1. Design Under Uncertainty.

This session will focus on the problem of designing and synthesizing continuous or batch processing systems in the presence of uncertainty. Uncertainty may be related to continuous and/or discrete process parameter variations,

equipment availability, environmental aspects, economic issues, etc. Topics of interest include, but are not limited to, metrics for characterizing uncertainty, approaches that introduce operability (e.g., flexibility, reliability, controllability) measures at the design stage, frameworks for plant operations under uncertainty, and process synthesis applications highlighting the impact of uncertainty on design decisions. Retrofit design applications are also welcome.

Chair

Sandro Macchietto
Dept of Chemical Eng. and
Chemical Technology
Imperial College
London SW7 2BY
UNITED KINGDOM
44-71-2258117
44-71-5819488 (FAX)

Co-Chair

Stratos Pistikopoulos
Dept of Chemical Eng. and
Chemical Technology
Imperial College
London SW7 2BY
UNITED KINGDOM
44-71-2258116
44-71-5819488 (FAX)

2. Design and Analysis.

Papers are solicited on recent developments in process design and analysis. Topics of interest include, but are not limited to, new process modeling methodologies, tailoring process models to design tasks, techniques for the design of specific units, design of integrated plants and systems, design and analysis under uncertainty or with incomplete data, generic design methods, and case studies in process design.

Chair

Michael L. Mavrovouniotis
Systems Research Center
University of Maryland
College Park, MD 20742
301-405-6620
301-314-9920 (FAX)
mlmavro@src.umd.edu

Co-Chair

Iftekhar A. Karimi
E.I. du Pont de Nemours & Co.
Waynesboro, VA 22980
703-946-1587
703-949-2949 (FAX)

3. Process Synthesis.

Papers describing original research in process synthesis are requested. Submissions describing new methodologies or significant new extensions or generalizations of existing approaches to process synthesis, or submissions describing the results of applications of existing synthesis methodologies are most appropriate for this session. Priority will be given to areas not covered in other sessions sponsored by CAST and to submissions of interest to the widest audience. Authors are requested to address these points in the extended abstract.

Chair

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

Co-Chair

Vivek Julka
Union Carbide Corporation
P. O. Box 8361
South Charleston, WV 25303
304-747-5949
304-747-5448 (FAX)

Joint Area 10a and Area 10d Session

1. Computational Approaches in Systems Engineering.

The increasing power of high performance computer architectures and further increases in the performance/price ratio of general-purpose computers continues to open up many new options for the use of computers as an aid for process systems engineers. This session will accept papers describing novel applications of computers in the context of the design, operation, management, or control of processes. Papers will also be accepted describing new algorithms, theory, or computational results in areas that affect the use of computers as a process support tool. These areas include artificial intelligence, differential systems, optimization, solution of nonlinear equations, etc.

Chair

Christodoulos A. Floudas
Dept of Chemical Eng.
Princeton University
Princeton, NJ 08544-5263
609-258-4595
609-258-2391 (FAX)
floudas@zeus.princeton.edu

Co-Chair

Joseph F. Pekny
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-7901
317-494-0805 (FAX)
pekny@ecn.purdue.edu

Joint Area 10a and Area 2 Session

1. Synthesis of Complex Separation Systems.

Chair

Vivek Julka
Union Carbide Corporation
P. O. Box 8361
South Charleston, WV 25303
304-747-5949
304-747-5448 (FAX)

Area 10b: Systems and Process Control

Note: This year the selection of papers for area 10b sessions will be based on review of abstracts and ranking after review. Each abstract will be sent to possibly 5 reviewers, their ratings will be averaged and ranked. Session chairs will finalize their sessions based on the rankings.

Oral presentations can be 15 or 20 minutes long, as decided by the session chairs.

All authors are strongly encouraged to provide manuscripts of their papers. If no manuscripts are available, copies of their audio visual materials must be distributed during the session. It is recommended that 4 transparencies or slides should be reduced and printed on one 8.5 x 11 paper. Thus, copies of 24 transparencies would fit on 3 pages (double sided). This reduction is also a good gauge for the size of lettering utilized in developing the visual aids. If after reduction to 25% your transparencies are not legible, your lettering is too small.

The list of sessions along with the names of session chairs is given below. Calls for papers will be issued by the session chairs soon. Please contact the session chairs and refer to their call for papers for further information about each session.

In keeping with the new guidelines adopted for paper submission at Area 10b sessions at AIChE meetings, potential presenters to this session are urged to send a completed PTP form and a 550-word abstract to the session chair AND six copies of the abstract to the CAST 10b Chairman, Prof. Ali Cinar, by March 2, 1993. Please state at the top of your abstract the title of the session. The abstracts will be sent out for review by Ali Cinar and the paper selection will be based on evaluation rankings.

If the research work has been presented previously, the authors are strongly urged to state in a paragraph how the proposed paper differs from the previous presentation(s) of the author(s).

Deadlines:

March 2, 1993 – Submit 550 word abstract (PTP). Send six copies to the CAST 10b chairman (Prof. Ali Cinar, address given below) AND one copy to a Session Co-Chair.

April 27, 1993 – Authors notified of acceptance.

Area 10b Chair:

Ali Cinar
Dept of Chemical Eng.
Illinois Institute of Technology
Chicago, IL 60616
312-567-3042
312-567-8874 (FAX)
checinar@minna.iit.edu

1. Advances in Process Control.

The object of this session is to provide a forum for presenting new and innovative techniques, methodologies and/or applications in process control. Papers that advance the state of the art in process control are sought. The main idea or theme of the paper to be presented should be clearly

described in the abstract. Priority will be given to areas not covered in the other process control sessions. Submit abstract to the Area 10b Chair at address noted above.

Chair

Babu Joseph
Chemical Engineering Dept
Washington University
St. Louis, MO 63130-4899
314-935-6076
314-935-4434 (FAX)
joseph@wuche2.wustl.edu

Co-Chair

Sigurd Skogestad
Chemical Engineering
Univ. of Trondheim – NTH
N-7034 Trondheim
NORWAY
47-7-594154
47-7-594080 (FAX)
skoge@kjemi.unit.no

2. Identification and Adaptive Control.

Topics of interest in identification include the use of Kalman filters and related techniques, neural networks, the on-line identification of nonlinear steady-state models, and the application of modulating functions. Adaptive control topics might include the stability of classical adaptive control algorithms, the use of neural networks, and fuzzy adaptive control. However, the session chairs are themselves adaptable to considering anything new or novel in this area. Submit abstract to the Area 10b Chair at address noted above.

Chair

Irvin H. Rinard
City College of CUNY
New York, NY 10031
212-650-7135
212-650-7193 (FAX)
rinard@che-mail.engr
.ccny.cuny.edu

Co-Chair

Thomas B. Co
Dept of Chemistry and
Chemical Engineering
Michigan Technological Univ.
Houghton, MI 49931
906-487-2144
906-487-2061 (FAX)
tbco@mtu.edu

3. Nonlinear Process Control.

Papers are solicited in the area of nonlinear process control. Papers discussing synthesis techniques (e.g., sliding mode control, I/O linearization, etc.) and emerging technologies (e.g., neural networks) are desired, particularly if they address robustness and practical implementation issues. Industrial case studies and papers that indicate when nonlinear control is most appropriate are also encouraged. Adaptive and model predictive approaches are discouraged, since these are covered in other sessions. Submit abstract to the Area 10b Chair at address noted above.

Chair

Daniel E. Rivera
 Dept of Chemical, Bio, and
 Materials Engineering
 Arizona State University
 Tempe, AZ 85287-6006
 602-965-9476
 602-965-2910 (FAX)
 rivera@asuvox.eas.asu.edu

Co-Chair

Francis J. Doyle
 School of Chemical Eng.
 Purdue University
 West Lafayette, IN 47907-1283
 317-494-9472
 317-494-0805 (FAX)
 fdoyle@ecn.purdue.edu

4. Model Predictive and Robust Control.

Papers are sought in the areas of predictive control and robust control. Contributions addressing robustness issues in predictive control schemes are of particular interest and will be given priority. However, a wider range of topics will also be considered. Key areas of the theory and application of Model Predictive Control strategies include stability analysis, assessment of performance limitations, tuning, synthesis, and multirate schemes. Key areas of Robust Control theory include robust synthesis for systems with multiple models or parametric uncertainties, robust and simultaneous stabilization and performance, robust control of constrained systems, and H-infinity, H-2, and l-1 designs. Submit abstract to the Area 10b Chair at address noted above.

Chair

Vasilios I. Manousiouthakis
 Dept of Chemical Eng.
 University of California
 Los Angeles, CA 90024-1592
 310-825-9385
 310-206-4107 (FAX)
 gilbert@ea.ucla.edu

Co-Chair

Oscar D. Crisalle
 Dept of Chemical Eng.
 University of Florida
 Gainesville, FL 32611
 904-392-5120
 904-392-9513 (FAX)
 crisalle@bitrun.che.ufl.edu

5. Solutions to the Industrial Challenge Problems in Process Control.

A number of realistic simulations of complex industrial processes were presented at a session titled "Industrial Challenge Problems in Process Control" at the 1990 AIChE annual meeting in Chicago. The control problems associated with each of these systems were described, but no solutions were offered. This present session will provide an opportunity for researchers to present their particular solutions to the challenge problems. While the focus of the session will be on control methods, new developments in analysis, identification, and on-line optimization as applied to the simulation systems will also be welcome. Papers describing experiences with the use of the simulation systems as teaching tools, for example, as project problems in undergraduate or graduate level courses, are also invited. Contributions from both industry and academia are welcome. Information on obtaining descriptions of the

challenge problems and the simulation code is available from the chairmen. Submit abstract to the Area 10b Chair at address noted above.

Chair

Randy C. McFarlane
 Amoco Research Center
 P. O. Box 3011
 Naperville, IL 60566-7011
 708-420-5760
 708-961-6250 (FAX)
 rcm@nap.amoco.com

Co-Chair

James J. Downs
 Eastman Chemical Co.
 P. O. Box 511
 Kingsport, TN 37662
 615-229-5318
 615-229-3966 (FAX)
 jjdowns@kodak.com

Joint Area 10b and Area 10c Poster Session**1. Issues in Process Modeling, Optimization, Monitoring, and Control.**

An important emphasis of this poster session will be on techniques and tools for monitoring process and control system performance and for detecting state changes and faults. For this poster session, monitoring and detection are defined broadly to include artificial intelligence, statistical, system theoretic, and integrated approaches. Data interpretation methodologies and approaches for generating states of unmeasured variables are also considered to be important elements of monitoring. Papers describing the performance of monitoring tools and techniques through case studies are particularly welcome. The authors should send one 500-word Abstract and a Proposal-to-Present form to one of the Chairs and six copies of the Abstract to Area 10b Chair Prof. Ali Cinar.

Chair

Yaman Arkun
 School of Chemical Eng.
 Georgia Inst. of Technology
 Atlanta, GA 30332-0100
 404-894-2865
 404-894-3120 (FAX)
 yaman_arkun@chemeng
 .gatech.edu

Co-Chair

Jay H. Lee
 Chemical Engineering Dept
 Auburn University
 Auburn, AL 36849-5127
 205-844-2060
 205-844-2063 (FAX)
 jhl@eng.auburn.edu

Co-Chair

Spyros A. Svoronos
 Dept of Chemical Eng.
 University of Florida
 Gainesville, FL 32611
 904-392-9101
 904-392-9513 (FAX)
 svoronos@pine.circa
 .ufl.edu

Co-Chair

James F. Davis
 Dept of Chemical Eng.
 Ohio State University
 Columbus, OH 43210-1180
 614-292-0090
 614-292-3769 (FAX)
 davis@kcgl1.eng
 .ohio-state.edu

Area 10c: Computers in Operations and Information Processing

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

(Cosponsored by the International Cooperation Committee of the Society of Chemical Engineers, Japan)

Contributions are sought describing methodological developments, implementations, and experiences with all aspects of CIM in the process industries. Subjects of particular interest include: integration of application areas such as plant information systems, monitoring, diagnosis, control, scheduling/optimization, planning, and design as well as developments within application areas themselves that focus on integration issues. Presentations of industrial experiences with CIM technology and critical discussions of limitations/advantages of current developments are also welcomed. Abstract should summarize the scope of the work, the methodology employed or developed, and significant conclusions and accomplishments.

Co-chair

Iori Hashimoto
Chemical Eng. Dept
Kyoto University
Yoshida-Honmachi Sakyo-ku
Kyoto 606
JAPAN
075-753-5567
075-752-9639 (FAX)
a52165@jpnkudpc.bitnet

Co-chair

G. V. Reklaitis
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-4075
317-494-0805 (FAX)
reklaiti@ecn.purdue.edu

2. Plant Wide Dynamic Simulation.

Papers are sought in the area of plant-wise dynamic simulation, namely the dynamic simulation of a large number of interconnected process equipment units. Topics of interest include applications such as operator training, plant-wide dynamic simulation at the process design stage, control system design, process safety, reliability and operability, and on-line dynamic simulation. Also of interest are technical advances in simulator development such as numerical solution algorithms, object-oriented programming, databases and other new programming techniques; parallel computing, client-server models, networks of workstations and other new computer architectures; general purpose simulation packages, and user interfaces. Deadlines: March 15, 1993, submission of two copies of a 500-word abstract to the session co-chairmen; April 1, 1993, authors informed of selection and session details; August 1, 1993, submission of an extended abstract; September 1, 1993, final manuscript due to the session chairman.

Chair

Jorge A. Mandler
Air Prod. & Chemicals Inc.
7201 Hamilton Blvd.
Allentown, PA 18195
215-481-3413
215-481-2446 (FAX)
mandleja@ttown.apci.com

Co-Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State University
Mississippi State, MS
39762-5623
601-325-2756
601-325-8997 (FAX)
tony@cs.msstate.edu

3. Artificial Intelligence in Process Engineering.

Contributions are solicited in the area of artificial intelligence applications in process engineering. Applications of AI to problems in fault diagnosis, supervisory control, scheduling, planning, and design as well as methodological contributions such as novel knowledge representation and/or reasoning techniques are welcome. Deadlines: March 15, 1993, submission of two copies of a 500-word abstract to the session co-chairmen; April 1, 1993, authors informed of selection and session details; August 1, 1993, submission of an extended abstract; September 1, 1993, final manuscript due to the session chairman.

Chair

Venkat
Venkatasubramanian
School of Chemical Eng.
Purdue University
West Lafayette, IN
47907-1283
317-494-0734
317-494-0805 (FAX)
venkat@ecn.purdue.edu

Co-Chair

Mark A. Kramer
Dept of Chemical Eng.
Massachusetts Institute
of Technology
Cambridge, MA 02139
617-253-6508
617-253-9695 (FAX)
mkramer@athena.mit.edu

4. Visualization in Chemical Engineering Systems.

This session will address issues arising from the use of computer imaging technology to visualize scientific and engineering data and information. As the quantities of such data (typically obtained via direct measurement and/or computer simulation) continue to increase, visualization techniques become vital to the comprehension and interpretation of these data. We solicit presentations on a variety of topics related to visualization, including, but not limited to, application areas for visualization methods, visualization techniques for complex data objects (e.g., higher dimensional tensor fields), animation, user interfaces and devices, data formats and transformations, and user interactions with simulation.

Area 10c: Computers in Operations and Information Processing

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

(Cosponsored by the International Cooperation Committee of the Society of Chemical Engineers, Japan)

Contributions are sought describing methodological developments, implementations, and experiences with all aspects of CIM in the process industries. Subjects of particular interest include: integration of application areas such as plant information systems, monitoring, diagnosis, control, scheduling/optimization, planning, and design as well as developments within application areas themselves that focus on integration issues. Presentations of industrial experiences with CIM technology and critical discussions of limitations/advantages of current developments are also welcomed. Abstract should summarize the scope of the work, the methodology employed or developed, and significant conclusions and accomplishments.

Co-chair

Iori Hashimoto
Chemical Eng. Dept
Kyoto University
Yoshida-Honmachi Sakyo-ku
Kyoto 606
JAPAN
075-753-5567
075-752-9639 (FAX)
a52165@jpnkudpc.bitnet

Co-chair

G. V. Reklaitis
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-4075
317-494-0805 (FAX)
reklaiti@ecn.purdue.edu

2. Plant Wide Dynamic Simulation.

Papers are sought in the area of plant-wise dynamic simulation, namely the dynamic simulation of a large number of interconnected process equipment units. Topics of interest include applications such as operator training, plant-wide dynamic simulation at the process design stage, control system design, process safety, reliability and operability, and on-line dynamic simulation. Also of interest are technical advances in simulator development such as numerical solution algorithms, object-oriented programming, databases and other new programming techniques; parallel computing, client-server models, networks of workstations and other new computer architectures; general purpose simulation packages, and user interfaces. Deadlines: March 15, 1993, submission of two copies of a 500-word abstract to the session co-chairmen; April 1, 1993, authors informed of selection and session details; August 1, 1993, submission of an extended abstract; September 1, 1993, final manuscript due to the session chairman.

Chair

Jorge A. Mandler
Air Prod. & Chemicals Inc.
7201 Hamilton Blvd.
Allentown, PA 18195
215-481-3413
215-481-2446 (FAX)
mandleja@ttown.apci.com

Co-Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State University
Mississippi State, MS
39762-5623
601-325-2756
601-325-8997 (FAX)
tony@cs.msstate.edu

3. Artificial Intelligence in Process Engineering.

Contributions are solicited in the area of artificial intelligence applications in process engineering. Applications of AI to problems in fault diagnosis, supervisory control, scheduling, planning, and design as well as methodological contributions such as novel knowledge representation and/or reasoning techniques are welcome. Deadlines: March 15, 1993, submission of two copies of a 500-word abstract to the session co-chairmen; April 1, 1993, authors informed of selection and session details; August 1, 1993, submission of an extended abstract; September 1, 1993, final manuscript due to the session chairman.

Chair

Venkat
Venkatasubramanian
School of Chemical Eng.
Purdue University
West Lafayette, IN
47907-1283
317-494-0734
317-494-0805 (FAX)
venkat@ecn.purdue.edu

Co-Chair

Mark A. Kramer
Dept of Chemical Eng.
Massachusetts Institute
of Technology
Cambridge, MA 02139
617-253-6508
617-253-9695 (FAX)
mkramer@athena.mit.edu

4. Visualization in Chemical Engineering Systems.

This session will address issues arising from the use of computer imaging technology to visualize scientific and engineering data and information. As the quantities of such data (typically obtained via direct measurement and/or computer simulation) continue to increase, visualization techniques become vital to the comprehension and interpretation of these data. We solicit presentations on a variety of topics related to visualization, including, but not limited to, application areas for visualization methods, visualization techniques for complex data objects (e.g., higher dimensional tensor fields), animation, user interfaces and devices, data formats and transformations, and user interactions with simulation.

Chair

Sangtae Kim
Dept of Chemical Eng.
University of Wisconsin
Madison, WI 53706-1691
608-262-5921
608-262-0832 (FAX)
kim@chewi.che.wisc.edu

Co-Chair

Alan B. Coon
Union Carbide Corporation
P. O. Box 8361
South Charleston, WV 25303
304-747-5470
304-747-5448 (FAX)
abc@abc@medinah.atc
.ucarb.com

Joint Area 10c and Area 10d Session

1. Parallel Numerical Methods and Applications.

Algorithms suitable for massively parallel computing (100+ computational-node systems) are extremely valuable to solving difficult problems in chemical engineering. This session will emphasize the derivation, verification, and use of numerical methods to massively parallel applications in chemical engineering. Applications should actually run on real parallel machines, not via simulation. Whenever possible, performance should be compared to competitive (perhaps non-parallel) solution approaches. Analysis of the scalability of such algorithms to larger problems (when relevant), and to large machine ensembles, should be considered. Fair comparisons of alternative parallel solution approaches as well as multiple machine architectures are encouraged. The presentation of new/modified numerical methods, with suitable justification, will also be considered, provided there is an intended application in chemical engineering and a clear connection is made. Such papers should indicate how parallelism is traded against stability in the formalism, and should preferably include experiments as well. Reference to related parallel algorithms research in other fields is encouraged, when relevant.

Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State University
Mississippi State, MS
39762-5623
601-325-2756
601-323-9729 (FAX)
tony@cs.msstate.edu

Co-Chair

Joseph F. Pekny
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-7901
317-494-0805 (FAX)
pekny@ecn.purdue.edu

Area 10d: Applied Mathematics and Numerical Analysis

1. Pattern Formation and Dynamics.

Our session will focus on experimental and theoretical investigations of temporal and spatial pattern dynamics in chemical systems. Examples that are of current interest

include solidification, heterogeneous and electrochemical reactions, multi-phase flow instabilities, and combustion.

Chair

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

Co-Chair

Yannis G. Kevrekidis
Dept of Chemical Eng
Princeton University
Princeton, NJ 08544-5263
609-258-2818
609-258-0211 (FAX)
yannis@marilyn.princeton.edu

2. Instabilities, Time Series, and Chaos.

Papers are sought dealing with single and multi-variable data manipulation and analysis of complex, possibly chaotic, systems of chemical engineering relevance described by ODEs or maps.

Chair

Julio Ottino
Dept of Chemical Eng.
Northwestern University
Evanston, IL 60208-3120
708-491-3558
708-491-3728 (FAX)

Co-Chair

B. Erik Ydstie
Dept of Chemical Eng.
Carnegie Mellon University
Pittsburgh, PA 15213

3. Self-Similarity, Scaling, and Renormalization in Chemical Engineering.

Papers are solicited which discuss self-similarity concepts in chemical engineering be it in connection with fractals, chaotic phenomena, or other processes in which analysis is facilitated through scaling or self-similar behavior.

Chair

D. Ramkrishna
School of Chemical Eng.
Purdue University
West Lafayette, IN
47907-1283
317-494-4066
317-494-0805 (FAX)

Co-Chair

Fernando J. Muzzio
Dept of Chemical and
Biochemical Engineering
Rutgers University
Piscataway, NJ 08855-0909

4. Probabilistic Models.

This session is generally concerned with the application of probabilistic concepts, stochastic simulation methods, and particularly in the area of dynamic stochastic modelling.

Chair

Kyriacos Zygourakis
Dept of Chemical Eng.
Rice University
Houston, TX 77251-1892
713-527-3509
713-524-5237 (FAX)
kzy%clio.decnet@
physics.rice.edu

Co-Chair

D. Ramkrishna
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-4066
317-494-0805 (FAX)

Call for Papers

ESCAPE-4

Dublin, Ireland, March 28-30, 1994

The ESCAPE symposia series is organized every year by the Computer Aided Process Engineering (CAPE) Working Party of the European Federation of Chemical Engineers. The most recent meetings were in Denmark (May 1992), Toulouse, France (October 1992) and Graz, Austria (July 1993, to be held).

ESCAPE-4 will be held in Dublin, Ireland on March 28-30, 1994. If you want to present a paper (either orally or as a poster) you should submit a 250 words abstract to:

ICHEME Conference Section (ESCAPE-4)
165-171 Railway Terrace
RUGBY Warwickshire CV21 3HQ
UNITED KINGDOM
Fax: (+44) 78 857 7182

Deadline abstract: March 17, 1993

Draft manuscript submission: July, 21 1993

Final manuscript submission: December 1993

First Call for CAST Sessions 1994 AIChE Spring National Meeting Atlanta, GA, April 17-21, 1994

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

September 1, 1993: Submit an abstract (camera-ready) on a completed original new-version AIChE Proposal-to-Present Form to the session chair and a copy also to the co-chair.

October 1, 1993: Session content is finalized. Authors are informed of selection.

January 1, 1994: Authors submit, if desired, any revision to the abstract (camera-ready) to AIChE.

March 1, 1994: Authors submit final manuscript to AIChE.

April 17, 1994: Speakers bring hard copies of visual aids to be distributed to the audience at the presentation.

Area 10a: Systems and Process Design

1. Computer-Aided Applications for the Pulp and Paper Industry.

This session will address recent developments in the area of computer-aided applications in the pulp and paper industry. Both theoretical and application papers are solicited in the areas of process simulation (steady state and dynamic), process design, process operation, increasing efficiency of units, separation systems, and waste management technologies. Papers with special interest to practicing engineers are particularly welcome.

Chair

Mahmoud El-Halwagi
Chemical Eng. Dept
Auburn University
Auburn, AL 36849-5127
205-844-2064
205-844-2063 (FAX)
mahmoud@eng.auburn.edu

Co-Chair

Harry Cullinan
Pulp and Paper Research
and Educational Center
Auburn University
Auburn, AL 36849

2. Process Synthesis.

Papers in process synthesis are being solicited including the synthesis of heat exchangers, reactors, mass exchange networks, separation systems, flowsheets, and synthesis for cleaner processes. Papers dealing with the analysis of

synthesized systems are also encouraged. Examples of analysis include stability and uncertainty issues, handling of process constraints, and convergence. Whenever possible, such papers should address implementation and other practical issues of interest to industrial practitioners.

Chair

Luke E. K. Achenie
Dept of Chemical Eng.
University of Connecticut
Storrs, CT 06268
203-486-4020
203-486-2959 (FAX)
achenie@uconnvm
.uconn.edu

Co-Chair

Stratos Pistikopoulos
Dept of Chemical Eng. and
Chemical Technology
Imperial College
London SW7 2BY
UNITED KINGDOM
44-71-2258116
44-71-5819488 (FAX)
e.pistikopoulos@ic.ac.uk

3-4. Design and Analysis I and II.

Papers are solicited which report on research results and their applications in the general area of design and analysis. Topics of interest include, but are not limited to, new models and design procedures for specific units, for subsystems, for whole plants, and for plant complexes; evaluation of such models and their sensitivity; and use of models with missing or uncertain data. Papers describing applications of new design or analysis methods are also appropriate. Preference will be given to papers not directly within the subject areas of other sessions sponsored by Area 10a at this meeting.

Chair

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

Co-Chair

Jeffrey J. Sirola
Eastman Chemical Co.
P.O. Box 1972
Kingsport, TN 37662-5150
615-229-3069
615-229-4558 (FAX)
sirola@kodak.com

5. Design of Batch Processes.

The last few years have seen batch processing emerge as an increasingly important mode of production for pharmaceuticals and other non-commodity chemicals. This session seeks papers that deal with all aspects of the design of batch processes including retrofit, the tradeoff between design and plant operating policy, design under uncertainty, new design strategies, heuristic methods, mathematical programming approaches, layout of batch plants, industrial case studies, tools for the support of batch design, and pipeless plant design.

Co-Chair

Iftekhhar A. Karimi
E.I. du Pont de Nemours
and Company
Waynesboro, VA 22980
703-946-1587
703-949-2949 (FAX)

Co-Chair

Joseph F. Pekny
School of Chemical Eng.
Purdue University
West Lafayette, IN 47907-1283
317-494-7901
317-494-0805 (FAX)
pekny@ecn.purdue.edu

6. Innovations in Process Modeling and Simulation.

This session on innovative applications of process modeling and simulation will have an emphasis on practical, yet creative ways of applying these tools to problems of commercial importance. The session will focus on applications and adaptations of existing tools to new or unique tasks including process synthesis, dynamic process modeling, etc., and also recent developments in modeling and simulation environments including applications of object-oriented programming techniques, equation-based simulations, and process data representation. Proposals to incorporate software demonstrations into the presentations are encouraged.

Chair

Robert S. Butner
Pacific NW Laboratory
P. O. Box 999
Richland, WA 99352
509-375-2675
509-375-2059 (FAX)
rs_butner@ccmail.pnl.gov

Co-Chair

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

Area 10b: Systems and Process Control

1. Model Predictive Control.

Papers emphasizing theory and practice of model predictive control including industrial applications, computer-aided design software are solicited.

Chair

Yaman Arkun
School of Chemical Eng.
Georgia Inst. of Technology
Atlanta, GA 30332-0100
404-994-2865
404-894-3120 (FAX)
yaman_arkun@chemeng
.gatech.edu

Co-Chair

F. Joseph Schork
School of Chemical Eng.
Georgia Inst. of Technology
Atlanta, GA 30332-0100
404-894-3274
404-894-2866 (FAX)
joseph_schork@chemeng
.gatech.edu

2. Modeling, Monitoring and Control in the Pulp and Paper Industries.

This session will provide a forum for the presentation and discussion of fundamental and applied studies in the areas of

modeling, instrumentation, and process control as they relate to pulp and paper industry problems. Topics of interest include, but are not limited to, process and system modeling, identification and inference, data reconciliation and process monitoring, nonlinear adaptive and model predictive control, and on-line implementation of statistical process control.

Chair

Ferhan Kayihan
Weyerhaeuser Techn. Ctr
Tacoma, WA 98477
206-924-6651
206-924-4380 (FAX)

Co-Chair

Robert R. Horton
Institute of Paper Science
and Technology
Atlanta, GA 30318-5794
404-853-9717
404-853-9510 (FAX)
robert.horton@ipst
.gatech.edu

3. Statistical Process Control.

Chair

Charles F. Moore
Dept of Chemical Eng.
University of Tennessee
Knoxville, TN 37996-2200
615-974-4326
cfmoore@utkux1.utk.edu

4. Empirical Process Modeling for Control.

Chair

Thomas J. Harris
Dept of Chemical Eng.
Queen's University
Kingston, ON K7L 3N6
CANADA
613-545-2772
613-545-6637 (FAX)
harrist@qucdn.queensu.ca

Co-Chair

Derrick K. Rollins
Dept of Chemical Eng.
Iowa State University
Ames, IA 50011-2230
515-294-5516
515-294-2689 (FAX)
drollins@iastate.edu

5. Novel Applications in Process Control.

Chair

Gerardo Mijares
M. W. Kellogg Company
P.O. Box 4557
Houston, TX 77210-4557
713-753-3014
713-753-5353 (FAX)

Co-Chair

Jonathan E. Withlow
Dept of Chemical and
Environmental Eng.
Florida Inst. of Technology
Melbourne, FL 32901-6988
407-768-8000 x-7354
407-984-8461 (FAX)

Area 10c: Computers in Operations and Information Processing

1. Environmental Considerations for Process Simulation and Operations.

Increased environmental awareness and regulation are precipitating the need to incorporate more environmental considerations into chemical process simulation and operations. This session will focus on the applications, trends, and challenges in end-of-pipe treatment methods, along with the identification of innovative pollution prevention opportunities during the plant design process. Topics of particular interest include process simulation tools and expert systems for considering environmental issues, dynamic simulation and stochastic modeling for solving environmental problems, handling of fugitive emissions and trace contaminants in simulation tools, process optimization with environmental objective functions, use of rate-based models for environmental calculations, better costing methods for environmental processes, and the incorporation of life-cycle analysis into process simulation and operations.

Chair

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

Co-Chair

Urmila Diwekar
Department of Engineering
and Public Policy
Carnegie Mellon University
Pittsburgh, PA 15213
415-268-3003
412-268-3757 (FAX)
ud01+@andrew.cmu.edu

2. Advances in Process Operations: Industrial Success Stories.

This session is for industrial practitioners to share experiences and case histories involving the implementation of computer-based or computer-aided operations support systems that have increased the productivity, profitability, or competitiveness of their processes. These systems may address problems such as data rectification, maintenance and reliability planning, fault detection, integration of optimization and operations, planning and scheduling, and supervisory control. The application of advanced technologies such as expert systems and neural networks are of particular interest. Also of interest are papers dealing with progressive management practices such as total quality management, not necessarily computer-based, which have been used successfully to improve process supervision and plant management. Priority will be given to papers describing actual case histories.

Chair

Mark A. Kramer
Dept of Chemical Eng.
Massachusetts Inst. of Technology
Cambridge, MA 02139
617-253-6508
617-253-9695 (FAX)
mkramer@athena.mit.edu

3. Techniques and Practice of Planning and Scheduling in Process Plants.

We are soliciting presentations on mathematical and heuristic techniques for planning and/or scheduling of process plants. Such techniques could include the application of control theory, mathematical programming, expert systems, artificial intelligence, man-machine techniques using interactive computer programs, use of data bases, etc. We are also soliciting expositions of planning and/or scheduling activities that are actually practiced in operating process plants. Such expositions may include explanations of data flows, human organizations, roles and functions of individuals and groups, and management processes including control of resources and activities. Finally, we are soliciting discussions of match and mismatch between theory and practice.

Chair

Michael T. Tayyabkhan
Tayyabkhan Consultants Inc.
62 Erdman Avenue
Princeton, NJ 08540
609-924-9174

4. Data Analysis for Process Applications.

Papers are solicited which address the different roles of data analysis in process engineering. The objective of the session is to share different ways in which process and/or laboratory data can be successfully manipulated and analyzed to solve problems of industrial significance. A broad range of applications is desired. Possible topics include, but are not limited to, estimation of thermophysical properties for commercial simulators, data analysis for model identification in predictive control, data analysis for product quality assurance, data driven fault diagnosis, pattern-based data analysis, model validation, and data validation.

Chair

Alan B. Coon
Union Carbide Corp.
P. O. Box 8361
South Charleston, WV 25303
304-747-5470
304-747-5448 (FAX)
abc@medinah.atc
.ucarb.com

Co-Chair

Rob Whiteley
School of Chemical Eng.
Oklahoma State Univ.
Stillwater, OK 74078-0537
405-744-9117
405-744-6187 (FAX)
whitele@master.ceat
.okstate.edu

5. Enabling Technologies for Next Generation Process Simulators.

Simulators that are much more elaborate mathematically and in software engineering terms are required for the future in process flowsheeting. The emerging need for dynamic simulation and the arrival of high performance computing (including massive parallelism) drive this need while providing new challenges. New computer science technologies (including object-oriented methods) and newer mathematical approaches (like Krylov sub-space iterative methods) are some of the things that can be brought to bear on such problems. Papers are sought that describe enabling technologies for next-generation process simulators and describe both the solved and yet-to-be-solved issues connected with their use. We are emphasizing revolutionary, rather than incremental, improvements with regard to software and associated efforts. Papers that discuss high performance architectures in connection with object-oriented solution strategies are especially welcome.

Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State Univ.
Mississippi State, MS
39762-5623
601-325-2756
601-323-9729 (FAX)
tony@cs.msstate.edu

Co-Chair

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

6. Application of High Performance Computing in Chemical Process Engineering.

High performance computing, in particular parallel computing and vector computing, has found applications in various areas of chemical process engineering, both industrial and academic. Among these areas are simulation, design, optimization, scheduling, and operation. Papers describing successful applications in such areas are sought. Papers are also sought that describe algorithms for efficiently exploiting vector and parallel architectures in such applications.

Co-Chair

Mark A. Stadtherr
Dept of Chemical Eng.
University of Illinois
Urbana, IL 61801
217-333-0275
217-244-8068 (FAX)
markst@turing.scs.uiuc.edu

Co-Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State Univ.
Mississippi State, MS
39762-5623
601-325-2756
601-323-9729 (FAX)
tony@cs.msstate.edu

Area 10d: Applied Mathematics and Numerical Analysis

1. Numerical Methods for ODE/DAE/PDEs.

We are arranging a session of four invited speakers, each of whom is a distinguished contributor to areas of research which have a significant impact on the numerical solution of ordinary differential equations, differential-algebraic equations, and partial differential equations. We plan to cover numerical methods and automatic codes for ODE/DAE/PDEs as well as automatic differentiation methods. This session will be of interest to practicing engineers who need to know how to build successful solution strategies based on available numerical software technology and algorithms.

Co-Chair

Anthony Skjellum
Dept of Computer Science
Mississippi State Univ.
Mississippi State, MS
39762-5623
601-325-2756
601-323-9729 (FAX)
tony@cs.msstate.edu

Co-Chair

Alan B. Coon
Union Carbide Corp.
P.O. Box 8361
South Charleston, WV 25303
304-747-5470
304-747-5448 (FAX)
abc@medinah.atc.ucarb.com

Call for Papers
ADCHEM '94
Kyoto, Japan, May 25-27, 1994

Scope

The Symposium will focus on methodologies for advanced process control. Papers highlighting industrial experience and/or comparisons between theory and practice are particularly welcome.

Dynamic Modelling and Simulation

Selection of model structure
Process identification, nonlinear regression
Sensitivity analysis, model validation
Computer-aided process modelling
Dynamic simulation techniques

Nonlinear Model-Based Predictive Control and Optimization

Nonlinear models and control objectives
Parameter and state estimation for control
Multi-objective and plant-wide control
Constrained optimization
On-line optimization techniques

Statistical Control Techniques

Process monitoring and supervision
Fault detection and diagnosis
PCA and PLS techniques
Model-based data reconciliation
Quality control

Knowledge-Based Versus Model-Based Control

Comparison of various control approaches such as fuzzy, neural-net-based or expert-system-based control with model predictive, adaptive, or robust control

Location

The ADCHEM '94 Symposium will be held at Kyoto Research Park. The International Symposium on Process Systems Engineering (PSE '94) will be held in Kyongju, Korea from

May 30 through June 3, 1994, i.e. immediately following ADCHEM '94.

Abstracts

The abstracts should, in 800–1000 words, formulate the problem and describe the methods used and the key results of the contribution. The authors must include a list of 4–5 keywords and also indicate for which topic area(s) the paper may be suitable.

Please send five copies of the abstracts in English to:

ADCHEM '94
Institut d'Automatique – DME
EPFL
CH-1015 Lausanne, Switzerland
Fax: +41-21-693-2574
e-mail: adchem@elia.epfl.ch

Deadlines

July 1, 1993: submission of extended abstracts

September 1, 1993: notification of conditional acceptance

November 1, 1993: submission of papers in camera-ready form

February 1, 1994: notification of final acceptance

ADCHEM '94 Secretariat

All correspondence (with the exception of the abstracts and papers) should be addressed to:

ADCHEM Secretariat
Department of Chemical Engineering
Kyoto University
Kyoto 606-01, JAPAN
Fax: +81-75-752-9639
e-mail: A52165@jpnkudpc.bitnet

**First Call for IFAC/ACC Workshop on the
Integration of Process Design and Control
Baltimore, MD, June 27–28, 1994**

The Workshop will be held in conjunction with the 1994 American Control Conference, on the Monday and Tuesday of the week of the ACC. (Application to IFAC to be submitted with ACC as NMO sponsoring the event.)

Workshop Theme

The existence of interactions between the design of a process and that of its control system have been known to industrial practitioners for a long time. In the past decade academic research has produced methodologies and tools that begin to address the issue of designing processes that are flexible, can be controlled reliably, and are inherently safe. The purpose of this Workshop is to bring together academics and practitioners with interests in the integration of process design and control, in order to examine the state of the art in methodologies and applications. Papers highlighting industrial experience or comparisons between theoretical predictions and experimental observations are particularly welcome. The scope of the Workshop will cover the design of chemical plants at different stages of detail. It will also examine control issues from the plantwide level, where, for example, recycles between units can be important, to the specific unit level, where the availability or selection of measurements might be the most important factor.

Some of the topics that will be considered are:

- Simultaneous process and control system design
- Controllability analysis
- Design for flexibility, resilience, and operability
- Design and control for inherent safety
- Structure selection of the process control system
- Optimization of process design and operation
- Measurement selection and availability
- Design and scheduling of batch plants
- Hazard and operability studies

Deadlines

September 15, 1993: Deadline for abstracts (400–600 words).

December 15, 1993: Authors to be notified about conditional acceptance.

March 1, 1994: Submission of papers in camera-ready form.

April 1, 1994: Notification of final acceptance.

Please send abstracts (5 copies) to the following address. All those interested in the Workshop are requested to indicate their interest by sending a note as early as possible.

Prof. Evangelos Zafiriou
Institute for Systems Research
A. V. Williams Building
University of Maryland
College Park, MD 20742
Fax: (301) 314-9920
e-mail: zafiriou@src.umd.edu

**Fifth Annual Real-Time Optimization in the Process Industries
An Industrial Short Course
June 7-10, 1993**

Real-time optimization (RTO) is one of the fastest growing areas of process control. RTO systems select the best values for plant operating variables based on current economics, sales demands, process performance and equipment capabilities. The course is intended for engineers with experience in design, operations or control; no prior optimization experience is assumed.

Goals

- Present the basic concepts of applied optimization with unique RTO issues
- Present best available technology for RTO with strengths and limitations
- Provide guidelines for successful selection and design of RTO applications
- Provide initial optimization experience through hands-on computer exercises

Outline

Overview of real-time optimization
Optimization fundamentals
Optimizing without an explicit model
Linear programming
Flowsheet case studies
Equation-based flowsheet optimization
Data reconciliation
Real-time implementation issues
Reduced order models

Simulation laboratories:

- Linear programming (steam system, blending)
- Flowsheet modelling (alkylation)
- Flowsheet optimization (alkylation, pulp & paper)
- Data reconciliation (ammonia plant)

Each student receives lecture notes, a simulation workbook, a Professional Demonstration version of GAMS and a disk with exercise files.

Dr. C.M. Crowe, Dr. A.N. Hrymak, and Dr. T.E. Marlin are all in the Department of Chemical Engineering at McMaster University. The instructors have over 40 years of experience in control and optimization and have published and consulted extensively.

For information contact Dr. Tom Marlin by telephone (416) 525-9140 ext. 7125 or by FAX at (416) 521-1350 or RTO Short Course, P.O. Box 20322, Upper James P.O., 858 Upper James St., Hamilton, Ontario, Canada L9C 7M8.

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Deadlines:

January 1 for Winter issue; July 1 for Summer issue.

Payment Details:

Prior to publication of advertisement, please submit check payable to CAST Division, AIChE, to the CAST secretary/treasurer: Dr. Lorenz T. Biegler, Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA 15213. Phone: (412) 268-2232. Fax: (412) 268-7139. Copy the editor, Dr. Peter Rony, on your letter of payment.

Editorial Department:

If you have questions, please contact Dr. Peter Rony, Editor, CAST Communications, at (703) 951-2805 (preferred, home phone) or (703) 231-7658 (leave message at work phone). Fax: (703) 231-5022. Email: RONY@VTVM1. His address is: Dr. Peter Rony, Department of Chemical Engineering, Virginia Tech, Blacksburg, Virginia 24061.