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Editorial Notes

by [Peter Rony](#)

Welcome to the second online-only issue of *CAST Communications* and the first formatted for web browsing. In May, this newsletter won the 2002 **Marx Isaacs Award for Outstanding Newsletter** from AIChE. We hope that this edition will be as well received and that this format will be easier to read and download than the previous full-issue pdf format.

Our two feature articles in this Summer 2002 issue are (1) the award address, ***Revolutions: All Sorts but Mostly Scientific***, given by Professor Christos Georgakis of the Department of Chemical Engineering, Chemistry, and Materials Science (Polytechnic University, Brooklyn, NY) and (2) ***An Industry Perspective on Polymer Process Modelling***, by Dr. Chau-Chyun Chen (Aspen Technology, Inc., Cambridge, MA), who respectively received the 2001 Computing in Chemical Engineering and the 2001 Computing Practice Award at the November 2001 CAST Division banquet in Reno, Nevada. These wonderful articles exemplify the unique role of *CAST Communications* as a publications medium in the AIChE. The editors thank both Professor Georgakis and Dr. Chen for taking the time to create and submit their articles to us. Christos' article took some time to create, but was well worth the wait.

Your editor heard both the thank you of Dr. Chen and Christos' award address in Reno last year. Both were special. We invite you to join us at the annual November banquet in Indianapolis.

And don't forget to read the [Quote of the Day](#).

Articles

REVOLUTIONS: All Sorts ... but Mostly Scientific

by Prof. Christos Georgakis



Bishop Blessing Soldiers; March 25, 1821

Abstract

In this paper, the author is expressing in written form the thoughts that he expressed orally last November at the CAST Division's dinner at the annual AIChE meeting in Reno, Nevada. The dinner presentation was prompted by his selection as the recipient of the CAST Division's Computing Awards. This paper examines the issue of revolutions and in particular scientific revolutions. Motivated by the work of Thomas Kuhn, the paper starts by discussing the four main paradigms that have characterized the development of Chemical Engineering. It then raises the question about what are the most important paradigms that characterize the Process Systems Engineering (PSE) community. A partial list of the possible PSE paradigms is presented and a question is raised whether they are as easily identifiable and widely accepted as the Chemical Engineering paradigms. The article ends with a suggestion that we should be aware of the global issues and concepts that affect our systems community, one of which is the transition that Chemical Engineering is experiencing now. This more global prospective will enable us to be more innovative and groundbreaking in our research activities and benefit from the new opportunities, rather than be bypassed by them. For those overly concerned with citations, a suggestion is offered in the postscript about which of the author's contributions are the most important.

 The [full article](#) [661 KB] may be downloaded in pdf format.

An Industry Perspective on Polymer Process Modeling

by Dr. Chau-Chyun Chen

Many chemical engineers dedicate their careers to process and product development, process debottlenecking, and process optimization for manufacturing plants. As they perform process studies, whether it is related to hydrocarbons, petroleum, chemicals, or polymers, they often apply process modeling technologies and tools to capture and apply the fundamental engineering understanding of the industrial processes. These tools for process modeling generally offer chemical engineers a robust and easy-to-use environment to develop and apply process models both quickly and productively.

Process modeling technologies and tools evolved over the past 30 years. Initially these technologies were primarily developed to meet the needs of the hydrocarbon and petroleum industries. The technology was then gradually expanded to address the needs of the petrochemical industry and, later, processes involving synthetic fuels (Gallier et al., 1984) and aqueous electrolytes (Chen et al., 1983; Chen, 1987).

Innovations in process modeling technologies and tools for the polymer processes evolved recently. The feasibility of modeling polymer processes with general-purpose process simulators was questioned as late as the early 1990s. However, key innovations in various polymer process modeling technologies have emerged and made it possible to develop high fidelity polymer process models that can be used for process design and

process optimization. As a result, the polymer industry has quickly and successfully adopted polymer process modeling technology.

This perspective highlights the unique challenges in polymer process modeling and the innovations that address these challenges. Also reported are the recent industrial applications of polymer process modeling technologies and tools that gradually came to wide acceptance in the past decade. Lastly opportunities for future innovations are suggested.

 The [full article](#) [150 KB] may be downloaded in pdf format.

LATEST NEWS: Majority of U.S. Population Now on the Web

New numbers from the U.S. Commerce Department indicate that in 2001, the number of Americans who use the Web passed the 50% mark for the first time. The report found that 143 million Americans, or 54% of the population, were using the Internet as of September. E-mail continues to be the favorite activity, regularly used by 45% of the population. The figures for young people aged 5-17 are especially noteworthy, with 90% now using computers. (*Wall Street Journal*, 4 Feb 2002)

Communications

2002 CAST Division Award Winners

by [Jay Lee](#) & [Karl Schnelle](#)

We would like to congratulate the three CAST Division Award winners for 2002. This communication includes short biographies, followed by selected quotations from supporting letters. The quotations were selected for their particularly strong impact. The awards will be presented at the upcoming AIChE Annual Meeting's CAST Award Dinner at Indianapolis.



Computing in Chemical Engineering Award: Manfred Morari, ETH, Zurich

For his pioneering contributions to the theory and applications of hybrid systems analysis and control, and his intellectual and professional leadership in Process Systems Engineering at large. Sponsored by The Dow Chemical Company & Mitsubishi Chemical Corporation.

In 1994 Manfred Morari was appointed head of the Automatic Control Laboratory at the Swiss Federal Institute of Technology (ETH) in Zurich. Before that, he was Professor of Chem Eng and Executive Officer for Control and Dynamical Systems at the California Institute of Technology. He obtained a Ph.D. from the University of Minnesota in Chem Eng. He has received numerous awards, among them the Allan P. Colburn Award and the Professional Progress Award from AIChE. In 1993 Prof. Morari was elected to the U.S. National Academy of Engineering.

Prof. Morari's research focuses on the development of methods for the analysis and design of control systems for complex and inaccurately known systems ("robust control"), and the investigation of the dynamics of nonlinear systems.

"The breath and depth of his work's impact, over the last 25 years, on the theory and practice of Process Systems Engineering, are monumental. He is the best of his generation. Broadening the scope to include control theorists across disciplines, [Manfred is one of] the top five in the world."

"He is such an obvious candidate. I really feel that his winning would be as much a compliment to the Award as the Award would be a compliment to him"

"His work has been very influential in determining the research agenda in process control during the last two decades. He has also developed an impressive school of former PhD students, some of whom are rapidly becoming established as leading members of the academic process control community in their own right."

"It is hard to think of other researchers in Process Systems Engineering who have had as much impact as Manfred has had."

"What is particularly impressive in my opinion is his ability to combine fundamental theoretical contributions with a keen interest in practical applications, as evidenced in his most impressive list of publications."



Computing in Practice Award: Marshall Rafal, OLI Systems, Inc.

For his outstanding accomplishments with regard to the creation of commercial software for the prediction of electrolyte-based process and corrosion simulation. Sponsored by Aspen Technology, Inc. and ExxonMobil Chemical Company.

Marshall Rafal is President of OLI Systems, Inc. in Morris Plains, NJ. Dr. Rafal attended Northwestern University where he received a Ph.D. in Chemical Engineering. He then worked for Esso Math & Systems, Inc. until founding OLI Systems in 1971. During the past 30 years, OLI has developed commercial computer software for simulating aqueous-based chemical systems. Dr. Rafal is a principal author of The Handbook of Aqueous Electrolyte Thermodynamics published by AIChE.

"Marshall is a rare individual whose combined technical and business contributions changed how the chemical industry simulates aqueous electrolyte equilibria and corrosion."

"The initial application of Dr. Rafal's software tools step-changed the technology of modeling aqueous electrolyte speciation. His diligence and constant quest for excellence have rendered tools which have become the world standard for calculation of speciation in aqueous systems."

"Marshall's commercial and scientific efforts in electrolyte thermodynamics have impacted many communities of researchers and for that alone he is very deserving of this award. The many communities include geochemists, chemistry, chemical engineering, biology and materials science and engineering to name a few."

"He has not only demonstrated high standards of academic pursuit in these fields of specialization, but also uniquely commercialized these different technologies into several easy-to-use OLI products."



Ted Peterson Student Award: Steinar Hauan, Carnegie-Mellon University

For fundamental insights leading to new synthesis methods for reactive distillation columns. Steinar has won the award for his paper "Phenomena based analysis of fixed points in reactive separations systems", Chem Eng Science, 1999. The work must have been done by the individual while pursuing graduate or undergraduate studies in Chemical Engineering. Sponsored by E.I. du Pont de Nemours and Company

Prof. Hauan completed his PhD in 1998 at the Norwegian Institute of Science and Technology and then took a post-doctoral position at the University of the Witwatersrand, South Africa. He is now an Assistant Professor of Chemical Engineering at Carnegie Mellon University. His current research interests include process design and analysis, mathematical modeling, and optimization.

"For discovering and understanding the implications of these geometric insights, Steinar is an excellent candidate. These are very important insights that help engineers understand how to design and when to use reactive distillation columns."

"Steinar Hauan's papers do for reactive distillation what McCabe and Thiele did for conventional distillation."

"One of the best results in reactive distillation was discovered by Steinar in his 1999 Chemical Engineering Science paper. This is a really beautiful result that can be used to develop a graphical interpretation of reactive azeotropes and to explain many of the design aspects of reactive distillation columns."

"Dr. Hauan has established himself as a leader in the development of geometric theories for chemical process design. His work is widely referenced and used."

"The main problem is understanding general regularities of reactive distillation at finite reflux. Steinar Hauan took an important step in this direction, using a geometrical approach to visualization..."

Introducing ChemVillage

One of the editors recently received this announcement, which may be of interest to other CAST members. As you will notice, no pricing is mentioned.

Dear Colleague,

Elsevier Engineering Information Inc. would like to introduce to you a breakthrough in desktop information delivery for the chemist and chemical engineer.

ChemVillage, The Intuitive Solution for Chemistry Research, is a powerful new search engine that allows you to search across multiple databases, quickly and seamlessly. Included in ChemVillage are two bibliographic databases, news, patents and handbooks from one easy-to-use interface.

A sample of some of the research tools in ChemVillage include:

Compendex Chemistry: Covers the top international chemistry and chemical engineering titles from 1998 to the present
Chemical Business NewsBase: Leading provider of worldwide chemical business news and information
Beilstein Abstracts: Access to over 600,000 abstracts and citations from the top journals in organic chemistry

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The following items are used to participate in the list:

1. To post messages to the list, please send mail to cast10@ench.umd.edu.
2. Subscribe/unsubscribe messages should be mailed to emailman@ench.umd.edu.
3. Archived messages can be found at www.ench.umd.edu/cast10.
4. Specific instructions on (un)subscribing and posting messages are located at www.ench.umd.edu/cast10/subscribe.shtml.
5. Include keywords as the first line of your message: **Keywords: software, jobs, education, meetings** using any or all of the keywords.

The list moderator, adomaiti@Glue.umd.edu, would like to invite comments on the operation of the e-mail list and archive website, especially suggestions for new services.

2003 Award Nomination Form

 The [form](#) [27KB] may be downloaded in WORD format. See [CAST Division Awards](#) for more information.

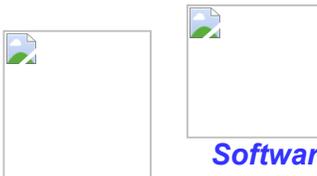
Quote of the Day

Among the devices that we use to impose order upon a complicated (but by no means unstructured) world, classification -- or the division of items into categories based on perceived similarities -- must rank as the most general and most pervasive of all. And no strategy of classification cuts deeper -- while providing such an even balance of benefits and difficulties -- than our propensity for division by two, or dichotomy. Some basic attributes of surrounding nature do exist as complementary pairings--two large lights in the sky representing day and night; two sexes that must couple their opposing parts to produce a continuity of generations -- so we might argue that dichotomization amounts to little more than good observation of the external world.

But far more often than not, dichotomization leads to misleading or even dangerous oversimplification. People and beliefs are not either good or evil (with the second category ripe for burning); and organisms are not either plant or animal, vertebrate or invertebrate, human or beast. We seem so driven to division by two, even in clearly inappropriate circumstances, that I must agree with several schools of thought (most notably Claude Levi-Strauss and the French structuralists) in viewing dichotomization more as an inherent mechanism of the brain's operation than as a valid perception of external reality."

Questioning the Millennium: A Rationalist's Guide to a Precisely Arbitrary Countdown
Stephen Jay Gould (1941-2002)

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Short Course for Industry

Learn marketable skills and help your company profit with our hands-on training for engineers, scientists, managers and techs: [Practical Process Control](#) - October 15 & 16, 2002

We begin this course with a firm foundation in the important fundamentals of PID control. We then move on to explore some of the advanced classical methods and techniques popular in current industrial practice. For all topics, you will gain hands-on experience in tuning controllers and testing algorithm performance.

The course is designed for a mixed audience including those who have had some training in the past and seek a refresher course, and those who have not had much formal training but desire to learn more. There is little math presented because we focus on how to use methods rather than how to derive them.

Day 1:

- Process Control Fundamentals
- Exploring Process Dynamic Behavior
- Process Data Collection and Analysis
- Tuning PID Controllers
- Nonlinear Behavior and Adaptive Control

Day 2:

- PID Tuning for Industrial Applications
- Optimizing Controller Performance
- Cascade Control Design and Tuning
- Feed Forward and Decoupling Control
- Model Based Smith Predictor for Dead Time Compensation

contact Doug Cooper at (860) 486-4092 or cooper@controlstation.com

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Deadlines:	December 1 for the Winter issue; July 1 for the Summer issue.
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Already a member? Please ask a colleague to join.

The Computing and Systems Technology (CAST) Division of AIChE is responsible for the wide range of activities within AIChE that involve the application of computers and mathematics to chemical engineering problems including process design, process control, operations, and applied mathematics. We arrange technical sessions at AIChE Meetings, organize special conferences, and publish this newsletter - *CAST*

Communications - twice a year. These activities enable our members to keep abreast of the rapidly changing fields of computing and system technology. The cost is \$10 per year, and includes a subscription to this newsletter. Shouldn't you join the CAST Division now?

To join the CAST Division, please contact AIChE Customer Service at the above address. You may also download and print [Join a Division or Forum -- 2002 Membership Application](#) from [AIChE](#).

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