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Computing and Systems Technology: AIChE® CAST



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CAST Communications - Fall 2004

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Editorial Notes on the "CAST Olympics"

by Peter Rony and Karl Schnelle

We invite CAST Division members who plan to attend the 2004 AIChE National Meeting in Austin, Texas to meet our three CAST division award winners -

Computing in Chemical Engineering Award winner, Ross Taylor (Clarkson University) for outstanding contributions to multicomponent mass transfer and for developing the non-equilibrium approach to separation process modeling and design;

W. David Smith, Jr. Graduate Student Publication Award winner, Sarette van den Heever (Decisive Analytics Corporation) for pioneering development of multiperiod mixed-integer nonlinear programming models and solution techniques for large-scale optimization of off-shore oil field infrastructures; and

Outstanding Young Researcher Award winner, Paul I. Barton (Massachusetts Institute of Technology) for pioneering contributions to theory, numerical methods, software development in dynamic modeling, simulation, optimization, and their application to a broad range of chemical and biological processes.

- at the CAST banquet on Tuesday evening. Also, please welcome our new 2005 CAST Division Officers: Karen A. High, Richard D. Braatz, and Oliver Smith.

More good news is that Panagiotis D. Christofides (UCLA) received the 2004 Donald P. Eckman Award given by the American Automatic Control Council. The Eckman Award is the highest honor for a young researcher, under the age of 36, in the field of automatic control. We thank the author, Sagar Gadewar (PDC Process Design Center, Inc.), of our feature article, "Current Trends in Conceptual Process Design", for contributing to CAST Communications.

The editors were captivated by the 24/7 coverage of the 2004 Olympics in the US. NBC and their associated cable channels seemed to cover many of the sports and even showed non-US winners! So we decided to do a little competition for ourselves. By coincidence, our first on-line newsletter was in 2000, so we compared our members' email addresses then and now.

Our winner is still .com over .edu. But there is a new player on the field: Mexico has moved up and replaced Korea in the listings! For those curious people, here is the year breakdown (%) by top level domain name (the rows sum to <100% because of the many domains with <1% each).

Year	.com	.edu	.net	.ca	.jp	.kr	.org	.gov	.mx
2000	59	19	7	2	2	1	1	1	<1
2004	56	20	11	3	1	<1	4	1	1

Please welcome a new advertiser, <u>I.r.partin enterprises</u>. And don't miss the <u>Quote of the Dav</u> on insanity and creativity.

Thirty-nine percent of respondents in an MSN survey have looked themselves up online, while just 36% reported using search engines to track down long-lost friends. The survey results indicate that many people are curious about how well-known they are, based on their personal websites, newsgroups and other web activity. The poll, conducted by Harris Interactive, also found that people spend 11 minutes combing through the results of a search, and 29% abandon their search without getting any useful information at all.

(<u>BBC News</u>, 4 Aug 2004)

Articles

Current Trends in Conceptual Process Design

Full article [440 KB]

by Sagar Gadewar, PDC Process Design Center Inc.

In recent years there has been a marked shift among the chemical companies away from bulk chemicals and towards high-value low-volume products. This shift has presented a number of challenges in applying the existing tools and methods for conceptual process design. Whilst there is some interest in improving existing tools, there is an increased need for the development of new tools that will aid in developing processes for manufacturing specialty chemicals, pharmaceuticals, and microstuctured products. In this paper, we will outline the current areas of interest in conceptual process design.

Conceptual design or "process synthesis" systematically generates potentially profitable alternatives based on the experimental and mathematical analysis of chemical routes to produce desired product/s from available raw materials. After remarkable progress in the past four decades, process synthesis is now a mature field. An outline of the history of the methods used for process synthesis was recently published in a retrospective article by Westerberg (2004).

The entire paper [440 KB] may be downloaded in pdf format.

2004 CAST Award Winners

by B. Wayne Bequette

We would like to congratulate the CAST Award winners for 2004. These three awards will be presented during the CAST Dinner at the 2004 AIChE Annual Meeting in November. This announcement includes short biographies and some notable quotations from the supporting letters.



Computing in Chemical Engineering Award: Ross Taylor, Clarkson University

For outstanding contributions to multicomponent mass transfer and for developing the non-equilibrium approach to separation process modeling and design. Sponsored by **The Dow Chemical Company & Mitsubishi Chemical Corporation**.

Ross Taylor is the Kodak Distinguished Professor of Chemical Engineering at Clarkson University in Potsdam, New York where he has been since 1980. He currently serves as chair of the Department of Chemical Engineering. He received BSc, MSc and PhD degrees from the University of Manchester, Institute of Science and Technology in England.

His research interests are in the areas of separation process modeling, multicomponent mass transfer, thermodynamics, and developing applications of computer algebra to process engineering (and cartography).

Prof. Taylor is the author or coauthor of over 70 refereed journal articles. He is a coauthor (with Prof. R. Krishna of the University of Amsterdam) of the textbook Multicomponent Mass Transfer (Wiley, 1993) and (with Dr. Harry Kooijman) of ChemSep, a software package that has been used in over 60 educational institutions around the world, as well as in industry. Prof. Taylor is also a trustee of The CACHE Corporation (Computer Aids for Chemical Engineering Education).

"His work has had a major impact on the models used for process analysis and design."

"[W]e have found immediate use for Ross's contributions in calculating condensation in the presence of inerts, vent scrubbing, and distillation, where there are large composition changes over a small number of trays. For an industry with a natural conservatism to trying new things, we have found Ross's work to have immediate adoption in some very important commercial processes."



W. David Smith, Jr. Graduate Student Publication Award: Sarette van den Heever, Decisive Analytics Corporation

For pioneering development of multiperiod mixed-integer nonlinear programming models and solution techniques for large-scale optimization of off-shore oil field infrastructures. Sponsored by **E.I. du Pont de Nemours and Company**.

Dr. Susara van den Heever earned her Ph.D. in Chemical Engineering from Carnegie Mellon University in 2001, and her Bachelor's degree in Chemical Engineering from the University of Pretoria, South Africa, in 1995. She is currently employed as an Operations Research Analyst at Decisive Analytics Corporation in Arlington, VA.

Her current research involves bidding strategies and bidder aid tools for combinatorial auctions, specifically as they relate to the FCC's spectrum auctions. Other research interests include strategic- and supply chain planning. Dr. Van den Heever has applied her research in the hydrocarbon, food and beverage, and telecommunication industries, in varying roles that include both technical and pre-sales consulting.

"Sarette is an innovator, who has successfully developed and applied novel solutions to extremely challenging problems in the oil and gas industry, which have been previously considered intractable."

"[T]his is the first concrete piece of work that addresses so efficiently and so innovatively the practical solutions of large-scale oilfield infrastructure planning models."



Outstanding Young Researcher Award: Paul I. Barton, Massachusetts Institute of Technology

For pioneering contributions to theory, numerical methods, software development in dynamic modeling, simulation, optimization, and their application to a broad range of chemical and biological processes.

Paul Barton is Associate Professor of Chemical Engineering at MIT, where he has been since 1992. He earned his M.Eng. (1988) and Ph.D. degrees (1992) from Imperial College, University of London. He has industrial experience with BP and Air Products.

Prof. Barton is currently serving as a Director of AIChE's Computing and Systems Technology Division. He is author or co-author of nearly 70 articles in refereed journals. He has been very active in the design and the development of process simulation software, having been the original author of gPROMS, and having led the development of ABACUSS and DAEPACK at MIT, all of which are now commercial products.

"He combines an originality of thinking with an attention to detail that, in my experience, are rarely found together in the same individual."

"(Paul's work on hybrid processes) has laid the theoretical foundations for much of our current capability for modeling, simulation, and optimization of such systems."

Communications

CAST Election Results

by Jimmy L. Humphrey and Karl Schnelle

We would like to congratulate the new CAST Second Vice-Chair and the two new CAST Directors.



2005 SECOND VICE-CHAIR: Karen A. High

Karen High is an Associate Professor in the School of Chemical Engineering at Oklahoma State University. She has been a faculty member at OSU since 1991. Karen has been active in the CAST division since 1991. She has served several times as session chair as well as presented papers for the CAST division. Most notably, she served as Director from 1997 to 1999. In addition to her responsibilities in Chemical Engineering, she served as the Coordinator of Women in Engineering from 1991 to 1996. From 1998 to 2001, Karen was the OSU site director for the Measurement and Control Engineering Center (MCEC) which is an NSF Industrial/University Cooperative Research Center. She continues to do research with the Center that is headquartered at the University of Tennessee at Knoxville.

Karen has received several OSU faculty awards for her dedication to education. Karen's main areas of interest include Economic Optimization in Control, Process Design and Optimization for Sustainability, Optimization of Industrial Catalytic processes and Creativity and Entrepreneurship in Engineering. Karen has had several National Science Foundation and industrial grants (primarily from ConocoPhillips) to support this research. She has predominantly taught process modeling, design, optimization, and numerical methods courses as well as Freshman Orientation courses at OSU.



2005-2007 DIRECTOR: Richard D. Braatz

Professor Braatz is Professor and University Scholar at the University of Illinois at Urbana-Champaign, where he holds joint positions in Chemical and Biomolecular Engineering, Applied Mathematics, Computational Science and Engineering, Bioengineering, the Beckman Institute, the Center for Nanoscale Science and Technology, and the National Center for Supercomputing Applications. His BS (1988) is from Oregon State University and his MS (1991) and Ph.D. (1993) are from California Institute of Technology. He spent a sabbatical at Massachusetts Institute of Technology (2002-2003).

Dr. Braatz is a co-author of 80+ journal papers and 3 books published by Springer Verlag including the textbook Fault Detection and Diagnosis in Industrial Systems. He has been highly active in CAST division activities, organizing and/or co-chairing over 25 sessions at AIChE and related conferences. He currently serves as the 2005 Program Coordinator for Area 10b and the AIChE Society Review Chair for the 2005 American Control Conference, and has contributed strongly to interactions between AIChE, IEEE, and IFAC including service on

numerous Program and Awards Committees. He currently serves as the Chair of the IEEE Technical Committee on Industrial Process Control and is an Associate Editor for the flagship IFAC journals, the Journal of Process Control and Automatica.



2005-2007 DIRECTOR: Oliver J. Smith

Dr. Smith received his Ph.D. in chemical engineering from Carnegie Mellon University and his B.ChE. from the University of Delaware. He is currently a Lead Process Engineer at Air Products and Chemicals Inc. where he has been employed since 1991.

Oliver has been instrumental in applying new leading edge computing technologies to actual problems in areas such as process synthesis, dynamic simulation, real-time optimization and process control. His use of novel dynamic control approaches in distillation start-up and novel modeling approaches in gas processing, has lead to five recent patents in these areas.

Panagiotis D. Christofides receives 2004 Donald P. Eckman Award by Jim Davis, UCLA



I am glad to announce that Professor Panagiotis D. Christofides of the Department of Chemical Engineering at UCLA recently received the 2004 Donald P. Eckman Award given by the American Automatic Control Council. The Eckman Award is the highest honor for a young researcher, under the age of 36, in the field of automatic control.

Panagiotis was cited for "pioneering contributions to analysis and control of nonlinear distributed parameter systems, accompanied by creative applications to advanced materials processing, particulate processes and fluid dynamic systems."

Information Technology in Chemical Engineering - Topical Conference

by Jimmy L. Humphrey

This year's topical at the <u>2004 Annual Meeting</u> is organized in a presentation and roundtable response to questions format. The focus will be on topics of most interest to chemical engineers in industry, university, and government. Topics include local, regional, national and international activities and case studies. Aggregation, compilation, exchange, and study of data will span across all topics. Discussion of innovative IT applications for research and development, new technologies and examples of where information technology can accelerate the development of new commercial businesses will occur.

More details are here.

How to Contact AIChE

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For answers to questions, try one of the following AIChE staff:

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Director of Technical Programming	Volunteer & Membership Activities
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	<u>Steve Smith</u> Director of Technical Activities & Journals (212) 591-7335

CAST10 E-Mail List

The following items are used to participate in the list:

- 1. To post messages to the list, please send mail to <u>cast10@ench.umd.edu</u>.
- 2. Subscribe/unsubscribe messages should be mailed to emailman@ench.umd.edu.
- 3. Archived messages can be found at <u>www.ench.umd.edu/cast10</u>.
- 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, <u>adomaiti@Glue.umd.edu</u>, would like to invite comments on the operation of the e-mail list and archive website, especially suggestions for new services.

2005 Award Nomination Form

The 2005 Award Nomination Form [16KB, PDF] should be completed by April 15. See CAST Division Awards for more information.

Quote of the Day

"Perhaps the most important ingredient of successful innovation is the creative technological idea that serves a pressing human need. This kind of creativity, in turn, requires a schizophrenic combination of rationality and insanity that's outside our ordinary experience. Imagine that all current inventions in the world and all their possible logical extensions and uses are inside a huge balloon. People are pretty good at extending these ideas further, using logical and common sense. But their results, being logical extensions of what's already there, stay within the balloon. To escape these, the balloon must be punctured with something that defies reason - a new idea that is akin to a form of insanity. Yet most insane ideas fail to be creative; they're simply insane. That's why successful innovators, after coming up with an idea that seems crazy, must be able to shift seamlessly to a rational dissection of the idea's merits and pitfalls. When this interplay between insanity and rationality converges, look out! A creative idea has been born."

Four Pillars of Innovation Michael Dertouzos (1936 - 2001)

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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 <u>Join a</u> <u>Division or Forum -- Membership Application</u> [30 KB, PDF] from <u>AIChE</u>.

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