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CAST Communications - Fall 2005

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Editorial Notes

by Peter Rony and Karl Schnelle

Welcome to the eighth online issue of CAST Communications. If you go to the URL http://www.castdiv.org/ArchivedNewsletters.htm, you will learn that our first online issue was the Summer 2002 issue. Also available at this URL are archived issues (in PDF format) of the newsletter dating back to Winter 1997. The editorial staff, which consists of Publications Board Chair and Editor, Peter Rony, and Associate Editor, Karl Schnelle, will continue serving the CAST Division for the next two years.

We congratulate our four CAST Division award winners:

Frank Doyle, Computing in Chemical Engineering Award winner;
Mike Morshedi, Computing Practice Award winner;
Martha Gallivan, the W. David Smith Jr. Graduate Student Publication Award winner, and
Richard Braatz, the Outstanding Young Researcher Award winner.

We also congratulate our new CAST Division Officers: **Gavin Towler**, our new Second Vice-Chair; **Karl Schnelle**, our new Secretary/Treasurer; **Dan Rozinski** and **Robert Young**, our new 2006-2008 Directors. Karl, who was just elected as the Division Secretary/Treasurer, has relinquished his role as Webmaster. **Matt Bassett**, the Area 10c Program Coordinator for 2006, has accepted the additional responsibility for maintaining the CAST website.

Photos and biosketches for our four winners and our newly elected members of the Executive Committee are given below.

We are especially proud to present Frank Doyle's Award address, "The Science of Control", at the CAST Division banquet on Tuesday evening in Cincinnati. Ignacio Grossmann, Jaime Cerdá, and Jose Pinto have done CAST members a favor through their summary of the virtual library on process systems engineering, which was developed in association with the PASI Conference on August 16-25, 2005.

Finally, Santanu Talukdar contributes an extensive article on regression coefficients and structural characterization of hydrocarbons in gasoline. We thank him for his contribution to this newsletter. And don't miss the Quote of the Day on serendipity.

Latest News - *"MT"*

If you still think that "MT" is only used to label compressed gas cylinders, then read on... The National Institute of Standards and Technology (NIST) announced results of its tests of several machine translation (MT) systems recently. The agency gave the top ranking to Google, not to university research programs or the standard Internet tool from Systran. Google used statistical analysis of word patterns to beat the traditional method of rule-based systems. To see why this is so important to the global chemical industry, take a look at the table in the news article.
(The Christian Science Monitor, 02 Jun 2005)

Articles

The "Science" of Control, Computing in Chemical Engineering Award Address
by Frank Doyle, UCSB


"Science" [3.2 MB]

For establishing process control principles in the field of systems biology, including control of complex biomedical systems, and analysis of regulation in biophysical networks.

Frank's entire address [3.2 MB] to the attendees of the 2005 CAST Awards dinner may be downloaded in pdf format.

Virtual Library on Process Systems Engineering from PASI Conference
by Ignacio Grossmann, Carnegie Mellon University; Jaime Cerdá, INTEC, Argentina; and Jose Pinto, Polytechnic University and University of Sao Paulo

The Pan American Advanced Studies Institute (PASI) on Process Systems Engineering took place on August 16-25, 2005, Iguazu Falls. The specific site for the workshop was the Hotel Cataratas in the Parque Nacional Iguazú, Argentina. The goal of the PASI on Process Systems Engineering, which was organized by Ignacio Grossmann, Jaime Cerdá and Jose Pinto, was to provide an advanced workshop that would bring together faculty and Ph.D. students from various countries in the Americas (U.S., Canada, Mexico, Argentina, Brazil, Chile, Colombia and Venezuela). Several students from Spain also participated. This workshop was also part of the activities of the CEPAC (Chemical Engineering Pan American Collaboration) group.

There were a total of 69 participants, and 21 lecturers and seminar speakers. The U.S. representation consisted of 25 Ph.D. students belonging to 21 universities: Auburn, Austin, Carnegie Mellon, Delaware, Florida, Georgia Tech, Illinois-Chicago, Illinois-Urbana, Lamar, Lehigh, Maryland, Northwestern, U. Pittsburgh, U. Pennsylvania, Penn State, Polytechnic, Princeton, Purdue, Rutgers, Texas A&M, Wisconsin (see list of participants). Funding was provided by the National Science Foundation and the Department of Energy. Matching funds were obtained from the Agencia Nacional de Promoción Científica y Tecnológica from Argentina, Carnegie Mellon University, Petrobras, Bayer and Honeywell (see sponsors)

A major objective of the PASI on Process Systems Engineering was to expose to the participants state-of-the-art developments in Process Systems Engineering in the following areas:

- Optimization
- Process and Product Design
- Process and Supply Chain Operations
- Process Dynamics and Control

There were a total of 12 modules in these areas, and each module was covered through a lecture lasting between 3 to 6 hours. There were also a number of one-hour seminars that complemented the lectures. A major outcome of the PASI conference was the development of *virtual library on Process Systems Engineering* that consists of the Powerpoint slides of the presentations, background articles, as well as exercises and MATLAB and GAMS computer files for various applications. The virtual library, found at http://cepac.cheme.cmu.edu/pasilectures.htm, contains the following topics:

Part 1. Optimization Modules

- Nonlinear and Dynamic Optimization, *Lorenz T. Biegler*
- Mixed-integer Optimization, *Ignacio E. Grossmann*
- Global Optimization and Optimization under Uncertainty, *Nikolaos V. Sahinidis*

Seminars:

- Dynamic modeling and optimization of large-scale cryogenic separation processes, *María Soledad Díaz*

Part 2. Process and Product Design Modules

- Biological pathways analysis and engineering, *Costas Maranas*
- Heat Integration, *Miguel J. Bagajewicz*
- Mass Integration and Pollution Prevention, *Mahmoud M. El-Halwagi*

Seminars:

- Water treatment network, *Juan Zamora*
- Synthesis of membrane processes for effluent treatment and metal recovery, *Ana Maria Eliceche*

- Disjunctive Programming: algorithms, implementation and solution of linear and non-linear models, *Aldo Vecchietti*
- Uncertainty analysis of process design and scheduling, *Marianthi Ierapetritou*

Part 3. Process and Supply Chain Operations Modules

- Batch Scheduling, *Jaime Cerdá*
- Supply chain optimization, *Jose Pinto*
- New product development, *Rex Reklaitis*

Seminars:

- Operations management in the fruit industry, *Alberto Bandoni*
- Constraint programming techniques for batch scheduling, *Gabriela Henning*.
- Synthesis of crystallization-based separation systems, *Luis Cisternas*
- Instrumentation Upgrade for Improved Process Monitoring, *Miguel J. Bagajewicz*

Part 4. Process Dynamics and Control Modules

- Advanced Process Dynamics and Control, *Oscar Crisalle*
- Model Predictive Control, *Jay H. Lee*
- Process Control Design, *Thomas E. Marlin*

Seminars:

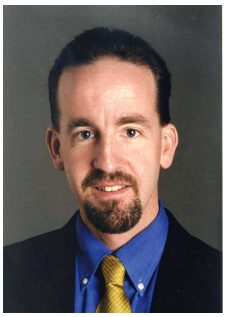
- Dynamic process simulation, *Argimiro Secchi*
- Robust control, *Darci Odloak*

Members of the CAST Division should hopefully find the material in this virtual library to be helpful. Practitioners will find useful overviews of areas that are of current interest and that are not normally found in textbooks and reference texts. The overviews emphasize the state-of-the-art in the corresponding area and are complemented by exercises. Academics should find the library useful for graduate level courses in Process Systems Engineering, and for introducing their students in the various research topics, as well as exposing them to various case studies. We intend to periodically update the presentations, and we will appreciate your feedback or comments.

Finally, we should conclude from our experience in this conference it was evident that Process Systems Engineering (PSE) is still very much an active and vibrant area of research in Chemical Engineering. Furthermore, it is clear that PSE continues to be of great industrial relevance as the scope of applications continues to grow, ranging from the molecular biological systems to specialty and large-scale commodity chemical plants, and all the way to the enterprise level. Our hope is that the virtual library will help to promote the interest in Process Systems Engineering.

2005 CAST Award Winners
by Karen High, 2005 CAST Second Vice-Chair

We would like to congratulate the CAST Award winners for 2005. These awards were presented during the CAST Dinner at the 2005 AIChE Annual Meeting in Cincinatti, OH, in November. This announcement includes short biographies and some notable quotations from the supporting letters.



Computing in Chemical Engineering Award: Frank Doyle, UC, Santa Barbara

For establishing process control principles in the field of systems biology, including control of complex biomedical systems, and analysis of regulation in biophysical networks. Sponsored by ***The Dow Chemical Company****.*

Dr. Frank Doyle holds the Duncan and Suzanne Mellichamp Chair in Process Control in the Department of Chemical Engineering at the University of California at Santa Barbara, as well as appointments in the Electrical Engineering Department, and the Biomolecular Science and Engineering Program. At UCSB, he is the Associate Director of the $50M Institute for Collaborative Biotechnology funded by the Army Research Office. Prior to his appointment at UCSB, he has held faculty appointments at Purdue University and the University of Delaware, and held visiting positions at DuPont, Weyerhaeuser, and Stuttgart University. His research interests are in systems biology, drug delivery for diabetes, and control of particulate processes.

"Frank's research on the reverse engineering of biological systems was innovative, high risk (very laudable for a young person at the start of his career!) and flashy…at UCSB Fran's career has taken a new turn…and he has been doing research at the forefront of systems biology."

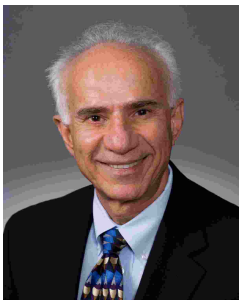
"Frank has established himself as the leading academic researcher in his age group in the area of biological process modeling and control, which arose out of a very productive collaboration with Dupont and other health-related companies."

"Frank's papers on control of glucose levels in the bloodstream by means of dynamic insulin delivery are first-rate, and the principles they elucidate and espouse could provide very helpful enhancements of drug delivery technology…"

"He contributed both to the model development for regulatory mechanisms, which must be seen as the enabling basis for all system theoretic work in this area, as well as to the development of system theoretic methods to analyze those systems."

Computing Practice Award, Mike Morshedi, PAS, Inc.

For contributions of fundamental technology and industrial-quality software for modeling, control, and optimization and for the development of QDMC for constrained Model Predictive Control. Sponsored by ***Aspen Technology, Inc. and ExxonMobil Chemical Company.****.*



With over thirty years of experience in the development and application of on-line optimization and control technologies, Dr. Mike Morshedi is one of the preeminent thought leaders and mathematical experts in the advanced process control industries worldwide. In 1980, Dr. Morshedi joined Shell Development Company where he became one of the principal developers of both OPERA and QDMC – industry's first equation-based optimizer and modern multivariable controller. As Chief Scientist at PAS, Dr. Morshedi leads a team of advanced application technologists focusing on soon-to-be-released next generation solutions that offer robust plant optimization and abnormal situation management concurrently.

"The impact of Mike's work on industrial practice has been evident, with major applications of Mike's software at many of the large oil refineries in the Houston area."

"Mike was instrumental in introducing the concept, benefits and techniques of open equation modeling to AspenTech...Mike's methods are used in virtually every real-time optimization application in operation today."

"Mike's early work with Shell Oil and resulting publications, has established him as one of the "founding fathers" of MVC…after Mike founded DOT-Products, Inc. he became the principle developer of a particularly novel formulation of MVC technology embodied in the STAAR Controller."

Outstanding Young Researcher Award: Richard Braatz, UIUC

For theoretical results in robust control, and their successful implementation in the paper, pharmaceutical, and other industries to increase product quality, reduce pollution, and conserve energy.

Dr. Richard Braatz is Professor and University Scholar at the University of Illinois at Urbana-Champaign, where he holds joint positions in Chemical and Biomolecular Engineering, Mechanical and Industrial Engineering, Bioengineering, Applied Mathematics, Computational Science and Engineering, and the Beckman Institute for Advanced Science and Technology. Dr. Braatz is a co-author of 90+ journal papers and 3 books published by Springer Verlag including the textbook Fault Detection and Diagnosis in Industrial Systems. In recent years Dr. Braatz has been investigating multiscale systems engineering, which is the simultaneous design and control of processes from molecular to macroscopic length scales.

"In the area of sheet forming processes, Prof. Braatz has pioneered new approaches for the control and identification…the second application is in the control of crystallization and particulate process applications."

"…he initiated new programs in the control of sheet and film processes, and in pharmaceutical crystallization. He has had a huge impact on both of these fields and continues to do so."

"Richard is by far the most cited process control researcher of his generation – and many of these citations come from outside chemical engineering."

"Richard's contributions in the general area of Control and Process Systems Analysis and in the particular area of "Robust control of complex, large scale systems" are truly deep and broad; the practical implications are also very significant indeed."

"Richard has addressed a series of real-world process control problems in ways that need to be highlighted for their inherent value. I am referring to his papers on the modeling, analysis and control of sheet and film processes (e.g. paper coating, polymer film extrusion) and batch crystallization."

W. David Smith, Jr. Graduate Student Publication Award: Martha Gallivan, Georgia Tech

For the journal paper, 'Reduction and Identification Methods for Markovian Control Systems, with Application to Thin Film Deposition,' with Richard M. Murray, *International Journal of Robust and Nonlinear Control*, **14**, 113-132 (2004). *Sponsored by* ***E.I. du Pont de Nemours and Company****.*

Dr. Martha Gallivan is an assistant professor in the School of Chemical & Biomolecular Engineering at Georgia Tech. Her graduate research was on the control of thin film deposition under the direction of Professors Richard Murray, David Goodwin, and Harry Atwater, and was supported by an NSF Graduate Fellowship. Professor Gallivan was the recipient of an NSF CAREER award in 2004, which supports computational and experimental research in chemical vapor deposition of metal oxide films for control of film microstructure. Her overall research program is on optimization and control of molecular-scale structure using self assembly with applications in inorganic crystalline films, polymer structure, and nanowire assembly.

"This is an important paper at the interface between atomistic/stochastic simulation and macroscopic systems theory and control."

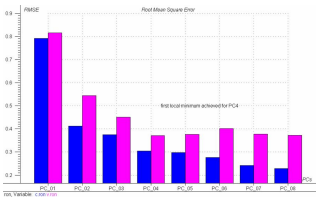
"What distinguishes this specific paper, aside from the high dimensionality of the model, is the treatment of the inherent stochasticity arising in microscopic-level models."

"My assessment of the paper's contributions is based on the innovative approach proposed in the paper for the simulation and model reduction of multiscale systems that are suitable for real time dynamic control and optimization."

"Martha's work is a landmark paper, one of the very first papers that successfully combines Kinetic Monte Carlo simulation with macroscopic control in a convincing manner."

Regression Coefficients and Structural Characterization Of Hydrocarbons In Gasoline
by Santanu Talukdar, Yokogawa India Ltd.

Santanu is an Engineering Services Manager, Analytical and Systems Engineering, and has been employed at Yokogawa India since 1997. His professional affiliations include AIChE, ISA, and IChemE. He holds a Bachelor's in Natural Science, University of Calcutta, India and a professional engineering diploma.



Full article [4147 KB]

In this application, a Fourier Transform Near InfraRed Analyzer (FT-NIR) is used to predict properties in Gasoline (Motor Spirit or MS). The predicted properties are given as a feedback to Advanced Process Control Software as Blend Property Control (BPC). The FT-NIR together with BPC and BRC (Blend Ratio Control) optimizes blending in the gasoline pool so that target values in final properties are achieved with minimum reblend and product giveaways.

Analysis is made on the basis of key structural characteristics in PIONA classification and its impact on property values.

In this study the key link between regression coefficients and structural characteristics of hydrocarbons is highlighted. The regression coefficients play a major role in prediction accuracy of the regression model developed. The step changes of the coefficients in terms of process recipe changes and process operating variable changes are highlighted.

The entire paper [147 KB] may be downloaded in pdf format. This paper uses Chemometrics and PLS techniques for data modeling. In an additional presentation [398 KB], PCA techniques for reducing error in the model are explained. Also, an overall tutorial on Chemometrics is in this presentation [460 KB].

Communications

CAST Election Results
by Oliver Smith, 2005-2007 CAST Director

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

2006 SECOND VICE-CHAIR: Gavin Towler

Dr. Towler is the Senior Manager of Process Design Development at UOP. In this role he leads a team of design engineers that is accountable for the design and optimization of all new process technologies developed by UOP, from conceptual design through to commercial implementation. He is also an Adjunct Professor at Northwestern University, where he co-teaches the design courses. Gavin has a B.A. and M.Eng. in chemical engineering from Cambridge University and a Ph.D. from U.C. Berkeley.

Gavin has been involved with CAST since he was in graduate school and has taken an active role in programming and chairing conference sessions for about ten years. He has chaired sessions for CAST in both the Annual and Spring National meetings and recently served as programming chair for systems and process design. He is interested in all aspects of process synthesis, design, optimization and control, and particularly in the application of new concepts to industrial practice. Gavin is also active in the national activities of AIChE and serves on AIChE's Membership Committee and the Chemical Technology Operating Council that oversees Divisions, meetings and publications. He has also been active in programming sessions for the Process Development and Fuels and Petrochemicals Divisions of AIChE

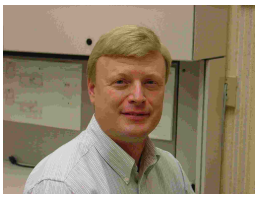
SECRETARY/TREASURER: Karl D. Schnelle

Dr. Schnelle is a Senior Scientist at Dow AgroSciences LLC in Indianapolis, IN. He received a BS degree from Vanderbilt University and a PhD degree in 1992 from Northwestern University, both in Chemical Engineering. Karl is a member of the mathematical modeling and analysis group of Dow AgroSciences R&D, where he develops and applies optimization, simulation, and statistical techniques to solve issues in R&D and manufacturing. Significant projects include prediction of environmental fate of agrochemicals, crop growth modeling, human health risk assessment, design and scheduling of manufacturing plants, supply chain planning, and advanced statistical analysis of batch plant data.

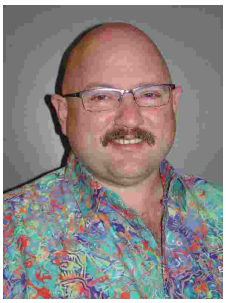
Since 1992, he has been a member of CAST. Currently, Karl maintains and updates the CAST website, is Associate Editor of CAST Communications, and helps run the CAST WebCASTs throughout the year. He was also a CAST Director for 2003-2005.

2006-2008 DIRECTOR: Dan Rozinski

Dan is a Manufacturing Execution Systems (MES) Project Leader at Rohm and Haas Company's corporate engineering division in Bristol, Pennsylvania. He is presently responsible for leading and



supporting MES strategies and projects throughout Rohm and Haas' thirteen businesses. Dan has a broad background, including chemical process and systems engineering with IBM, engineering and manufacturing application support with Aspen Technology, manufacturing technology strategy at Hercules, and most recently leadership for plant to business integration initiatives within Rohm and Haas. Dan has over 18 years of experience in driving business value from engineering and manufacturing technology, from both the solution supplier and operating company perspective.



2006-2008 DIRECTOR: Robert Young

Robert is currently the Advanced Control Section Supervisor at ExxonMobil's Torrance Refinery in Torrance, CA. He has been with ExxonMobil Refining and Supply since 2001 and ExxonMobil Chemical Company since 1991. Prior his employment at ExxonMobil, he was employed by ICOTRON as Process Control Engineer and Consultant. His BS degree (1983) is from the University of Texas - Austin, and his MS degree (1985) and Ph.D. (1988) are from University of California Santa Barbara.

Dr. Young has both lead and implemented a wide variety of process control projects in the areas of linear and nonlinear multivariable predictive control, polymerization reactor control, process control system replacement, and manufacturing execution systems. In addition, Dr Young has also providing process control support for several operating facilities. He is a co-author of 14 journal and technical meeting papers and presentations and is the co-inventor on a patent relevant to the control of polymerization reactors. He has been active in CAST Division activities, organizing and/or co-chairing sessions at AIChE and related conferences. He is currently serving as the 2007 Program Coordinator for Area 10b and the AIChE Society Review Chair for the 2007 American Control Conference. Robert is a member of AICHE, IEEE, and SIAM. He actively participates in university consortia such as the Texas Wisconsin Modeling and Control Consortium.

How to Contact AIChE

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Joe Cramer Director of Technical Programming (212) 591-7950	Anette Ngijol Volunteer & Membership Activities (212) 591-7478
Sarah Fewster Manager, Communications 212.591.7527	Steve Smith Director of Technical Activities & Journals (212) 591-7335

CAST10 E-Mail List

The following websites are used to participate in the list:

1. lists.isr.umd.edu/mailman/listinfo/cast10 is the link subscribers (current and new) can use to manage their subscription properties.
2. www.ench.umd.edu/cast10/ has lots of archive information and background information. The preferred address to post messages to the list is cast10 at ench.umd.edu.

2006 Award Nomination Form

The 2006 Award Nomination Form [17KB, PDF] should be completed by April 15. See CAST Division Awards for more information.

Quote of the Day

"I once read a silly fairy tale, called *The Three Princes of Serendip*: as their Highnesses travelled, they were always making discoveries, by accidents and sagacity, of things which they were not in quest of: for instance, one of them discovered that a mule blind of the right eye had travelled the same road lately, because the grass was eaten only on the left side, where it was worse than on the right—now do you understand Serendipity?"

Letter to Sir Horace Mann, 28 Jan. 1754
Horace Walpole (1717 - 1797)

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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 -- Membership Application [30 KB, PDF] from AIChE.

CAST Communications - Fall 2005
The Semi-Annual Publication of the Computers and Systems Technology Division of AIChE
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Associate Editor: Karl D. Schnelle, Dow AgroSciences LLC