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CAST Communications - Summer 2013

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Editorial Notes

by Peter Rony and Karl Schnelle

Welcome to the Summer 2013 issue of *CAST Communications*.

This issue is packed with 2012 CAST Division activities that demonstrate the value of an online newsletter. To summarize, we provide the results of the 2012 CAST elections; the winner and honorable mentions of the 2012 CAST director's award; bio-sketches for the seven 2012 CAST award winners; a PDF file for the award lecture introduction by B. Wayne Bequette, who, in our opinion, continues to be CAST's version of Bob Hope; the PDF file for the 2012 Computing in Chemical Engineering award lecture; photos of the 2012 CAST poster session and awards dinner; the five winners of the 2012 CAST travel awards; the 2012 CAST director's student presentation award; how to contact the AIChE; CAST awards nomination form; quote of the day; and finally, the *CAST Communications* advertising policy. We congratulate all of our award winners and thank Marianthi Ierapetritou for her images of the 2012 poster session and Ray Adomaitis for his images of the CAST Awards Dinner.

And the [Quote of the Day](#) is by John Steinbeck.

Articles

History of *CAST Communications*

by Peter Rony, Publications Board Chair

This is the final issue that is co-edited by Karl and myself. As editor of *CAST Communications* for 27 years, I believe that a bit of history is appropriate here.

Edward Rosen, 1985 chair of the CAST division, invited me to become the editor of the CAST newsletter. I accepted Ed's invitation and, within a year or two, altered the printed newsletter from a publication that published only the CAST session agendas (for the spring and fall AIChE meetings) into a printed newsletter, *CAST Communications*, that became both the flagship publication and archival newsletter of the CAST division.

I have **Joe Wright** (Xerox Corporation, Canada) to thank for his significant role in the early years of the newsletter. As editor, I was responsible for the acquisition of content, including bio-sketches of CAST award winners, original articles, a listing of forthcoming professional meetings, and the CAST-Division-Award winner's presentation at the November CAST dinner. As producer, Joe was responsible for taking the content and formatting it into a newsletter. As printer, AIChE headquarters printed the newsletter and mailed it to the CAST members. Each mailed CAST newsletter cost the CAST division between \$1500 and \$2000 in printing and postage costs.

I have been supported over the decades by associate editors **Joe Wright [1985-1994]**, **Scott Keeler [1995-1999]**, and **Karl Schnelle [2000-2013]**, whose contributions to the continuing success of the newsletter were (and are) outstanding.

Because the \$2000-per-issue cost weighed heavily on both Karl and myself, in 2000, we transitioned the newsletter into an online publication. This transition presented two significant benefits: (1) no printing and mailing cost, and (2) our ability to include color images. At the time, we were concerned about the possible displeasure of our membership to such a transition. We were mistaken. The rest is history.

CAST Communications has received the AIChE Max Isaacs award for the outstanding division newsletter three times. Every issue of this newsletter is archived [here!](#)

Videos in Honor of Manfred Morari's 60th Birthday

by Richard D. Braatz and Jay Hyung Lee

Two special sessions in honor of Manfred Morari's 60th birthday were held on October 17, 2011 at the AIChE Annual Meeting in Minneapolis, Minnesota. Presentations were given by George Stephanopoulos, W. Harmon Ray, Ignacio E. Grossmann, Lorenz T. Biegler, Tariq Samad, Thomas F. Edgar, Carlos E. Garcia (with input from Daniel Rivera), Sigurd Skogestad, Jay H. Lee (with input from Mayuresh V. Kothare), Francis J. Doyle III, Francesco Borrelli, and Manfred Morari.

Videos of these oral presentations are now available on an [open website](#).

Communications

2012 CAST Election Results

by Karl Schnelle, CAST Secretary

The CAST Executive Committee is pleased to announce the results of the election of officers for 2013. Results for 2014 will be announced shortly.

Please join us in congratulating our new Second Vice-Chair and two new Directors. Two new Directors are elected every year to serve a three year term. The CAST Secretary/Treasurer is elected every two years.



SECOND VICE-CHAIR: Raymond A. Adomaitis

Ray Adomaitis received his B.S. and Ph.D. in Chemical Engineering from the Illinois Institute of Technology. After two years working on computational nonlinear dynamics as a postdoctoral researcher at Princeton University, he joined the Institute for Systems Research (ISR) at the University of Maryland as a postdoctoral fellow. Currently, he is a Professor and Associate Chair for Undergraduate Studies in the Chemical and Biomolecular Engineering Department with a joint appointment at the ISR at the University of Maryland. He also is affiliated with the Maryland Nanocenter and the University of Maryland Energy Research Center (UMERC).

Ray's research and teaching interests focus on simulation and design of thin-film manufacturing processes with applications in microelectronics, alternative energy, nanomanufacturing, and spacecraft systems. Most of his current efforts are directed to developing physically-based models of atomic layer deposition surface reaction kinetics to provide simulation tools for the scale-up of these processes to large-substrate formats. Ray has been an active member of the executive committees of the CAST division and National Capital section of AIChE, and more recently as a member of the AIChE Public Affairs and Information Committee. He is a fellow of the AIChE.



2013-2015 DIRECTOR: John R. Richards

Dr. John R. Richards, P.E. is a Research Fellow in DuPont Engineering Research and Technology at the Experimental Station in Delaware, and has worked on various processes and plant sites that employ polymerization and biological modeling and process control. He has developed polymerization models and control systems for a broad spectrum of products and processes, including polymers, monomers, and biological systems, all of which have resulted in a significant impact in terms of improved yield, quality, and productivity. He has been the recipient of three DuPont Engineering Excellence Awards.

He is an Affiliated Faculty member of Chemical Engineering at the University of Delaware where he has taught the Fundamentals of Engineering and Professional Engineering Review in Chemical Engineering courses since 1983. He has authored 21 publications in refereed journals, a book, 6 book chapters and theses and 38 conference presentations.

An AIChE member since 1976, he organized sessions at Annual AIChE and ACC Meetings on "Modeling and Control of Polymer Processes" every other year from 2002 to 2012. He was Conference Industrial Co-chair at the 2009 Polymer Reaction Engineering (PRE) VII, the premier PRE conference that is held every three years. He was elected an AIChE Fellow in 2011. He was awarded the CAST Computing Practice award in 2012. He is an Educational Associate at the Mount Cuba Astronomical Observatory.

He received his BS in Biochemical Engineering and AB in Psychology from Rutgers University in 1976 and his MS from Cornell University in Chemical Engineering in 1978. He then joined DuPont and received his PhD from the University of Delaware in Chemical Engineering in 1994.



2013-2015 DIRECTOR: Carl Laird

Carl Laird, assistant professor in the Artie McFerrin Department of Chemical Engineering at Texas A&M University, is holder of the Ruth and William J. Neely '52 Faculty Fellowship. Dr. Laird's research interests include large-scale nonlinear optimization and parallel scientific computing. Focus areas include chemical process systems, homeland security applications, and large-scale infectious disease spread. Dr. Laird is the recipient of several research and teaching awards, including the prestigious Wilkinson Prize for Numerical Software and the IBM Bravo award for his work on IPOPT, a software library for solving nonlinear, nonconvex, large-scale continuous optimization problems. He is also a recipient of the National Science Foundation Faculty Early Development (CAREER) Award and the Montague Center for Teaching Excellence Award.

Dr. Laird earned his Ph.D. in Chemical Engineering from Carnegie Mellon in 2006 and his Bachelor of Science in Chemical Engineering from the University of Alberta.

Secretary/Treasurer: Karl D. Schnelle



Karl D. Schnelle is a Senior R&D Scientist at Dow AgroSciences LLC. He received a BS degree from Vanderbilt University, and then received a PhD degree in Artificial Intelligence Applications in 1992 from Northwestern University – both in Chemical Engineering.

Prior to his PhD, Karl had worked as a process engineer for DuPont. Currently, he is transitioning from a Senior Research Leader in R&D Analytics to a role as Master Black Belt in Strategic Planning and Operations at Dow. Karl also provides leadership across R&D so that researchers are well trained in design of experiments and statistical analysis of data.

2012 CAST Directors' Award

By Robert S. Parker, CAST Director

Recognizes the presenter of a poster at the annual meeting judged as outstanding by the CAST directors.

It is our pleasure to announce the winner of the Directors' Award for the Best Poster at the 2012 AIChE Annual Meeting.

The winner of the Directors' Award is:

First Place: **Curtisha D. Travis**, University of Maryland, "The Computational Challenges of Simulating Atomic Layer Deposition (ALD) Process Dynamics" ([Abstract](#))

Curtisha is a chemical engineering PhD candidate, working with Dr. Raymond A. Adomaitis, and is slated to complete her degree in December of 2013. She earned a bachelor's degree in chemistry with a minor in mathematics from Howard University and thereafter earned a standard instructional certificate to teach K-12 chemistry from Seton Hall University as a Teach For America and AmeriCorps member. Curtisha spent two years teaching high school chemistry and general science in Newark, NJ prior to beginning graduate school at the University of Maryland where her research focuses on modeling the surface reactions, film growth, and reactor transport dynamics in atomic layer deposition processes. Upon obtaining her PhD, Curtisha hopes to first begin a career in industry that continues her emphasis on thin films. During that time she hopes to partner with universities and local communities to build and sustain STEM pipeline programs for under-represented minority students, and perhaps transition back into academia at a later time.



Honorable Mention: **Arul Sundaramoorthy**, James M. B. Evans, and Paul I. Barton; "Capacity Planning in Novel Pharmaceutical Supply Chains under Clinical Trials and Demand Uncertainties"

Honorable Mention: **Sean Legg**, Alberto Benavides-Serrano, M. Sam Mannan, and Carl D. Laird; "Optimal Placement of Gas Detectors in Process Facilities Using Conditional Value At Risk"

Honorable Mention: **Mo Jiang**, Xiaoxiang Zhu, Mark Molaro, Michael L. Rasche, Davide M. Raimondo, Kwang-Ki Kim, Haitao Zhang, Keith Chadwick, Lifang Zhou, Zhilong Zhu, Minhao Wong, Des O'Grady, Dominique Hebrault, John Tedesco and Richard D. Braatz; "Multidimensional Population Balance Model for Growth and Dissolution Identified from a Designed Temperature-Cycling Experiment"

Photos of all the posters are [here](#).

2012 CAST Award Winners

by Marianthi Ierapetritou, 2012 CAST Second Vice-Chair

COMPUTING IN CHEMICAL ENGINEERING AWARD



Efstratios (Stratos) Pistikopoulos is the recipient of the Computing in Chemical Engineering Award for contributions to process design and operations under uncertainty, multiparametric model predictive control, and industrial applications. This award recognizes outstanding contributions in the application of computing and systems technology to chemical engineering, and is sponsored by The Dow Chemical Company. He is Professor and Director of Research in the Department of Chemical Engineering at Imperial College London. Stratos received his PhD from Carnegie Mellon and Diploma from Aristotle Univ. of Thessaloniki. His research covers the areas of modeling, control, and optimization of process and systems engineering applications.

COMPUTING PRACTICE AWARD



John Congalidis and John Richards are the recipients of the Computing Practice Award for the development and application of fundamental models of polymerization reactors and control strategies that result in enhanced quality, yield, and reduced time from laboratory to manufacturing. This award recognizes outstanding contributions in the practice or application of chemical engineering to computing and systems technology, and is sponsored by Aspen Technology, Inc. and ExxonMobil Chemical Company.

John Congalidis was a Research Planning Manager with DuPont Central Research and Development. He received his PhD from MIT and BS from NTUA. His career with DuPont included assignments in advanced process control systems implementation, polymer products development and manufacturing, kinetic modeling, strategic planning, and research management. *It is with sad news that we report that our colleague, Dr. John Congalidis, passed away on January 17, 2013.*



John Richards is a Research Fellow in DuPont Engineering Research and Technology at the Experimental Station in Delaware. He received his MS from Cornell, and BS from Rutgers Univ. John has worked on various processes and plant sites, employing polymerization and biological modeling and process control.

OUTSTANDING YOUNG RESEARCHER AWARD



Christopher Rao is the recipient of the CAST Outstanding Young Researcher Award for contributions to control theory and multi-scale simulation and their application to biological systems. This award recognizes an individual under the age of 40 for outstanding contributions to the chemical engineering computing and systems technology literature and is sponsored by Air Products. Chris is Associate Professor of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign. He received his PhD from University of Wisconsin, Madison and BS from Carnegie Mellon University. His postdoctoral work was at University of California, Berkeley and the Howard Hughes Medical Institute. Research interests include systems and synthetic biology, with a specific interest in understanding how cells employ feedback control in decision-making processes.

DAVID HIMMELBLAU AWARD



David Kofke and Andrew Schultz are the recipients of the David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education for the development of the etomica modules, a community-developed suite of interactive simulations to help students understand the molecular origins of macroscopic behaviors. This award recognizes an individual or group making new and novel contributions to computer aids for chemical engineering education, and is sponsored by the Chemstations.

David is a UB Distinguished Professor. He received his PhD from Univ. of Pennsylvania and BS from Carnegie Mellon University. He works in development and understanding of molecular simulation methods.



Andrew is a Research Assistant Professor at the University of Buffalo. He received his PhD from North Carolina State Univ. and BS from University of Tulsa. His research interests include development and application of methods in molecular simulation and statistical thermodynamics.

DAVE SMITH JR. GRADUATE PUBLICATION AWARD



Yoshiaki Kawajiri is the recipient of the W. David Smith, Jr. Graduate Publication Award, which recognizes an individual for published work on the application of computing and systems technology to chemical engineering, and is sponsored by Process Systems Enterprise Limited. Yoshiaki has been an Assistant Professor at Georgia Tech since 2008. He received his PhD from Carnegie Mellon University. Postdoc work was completed at the Max Planck Institute for Dynamics of Complex Systems in Magdeburg, Germany as an Alexander von Humboldt Research Fellow. His research is in the areas of modeling, design, and optimization of separations processes. Publication: "Optimization Strategies for Simulated Moving Bed and Power Feed Processes", **AICHE Journal** 52(4), 2006, with Larry Biegler.

Award Lecture Introduction

by B. Wayne Bequette, CAST Division Past Programming Chair

Computing in Chemical Engineering Award - *Recognizes outstanding contributions in the application of computing and systems technology to chemical engineering*

Wayne presented an [introduction](#) [1.8MB] to the attendees of the 2012 CAST Awards Dinner. *Warning: Some photos contained in this pdf are not suitable for all audiences!*



[source: rpi.edu]

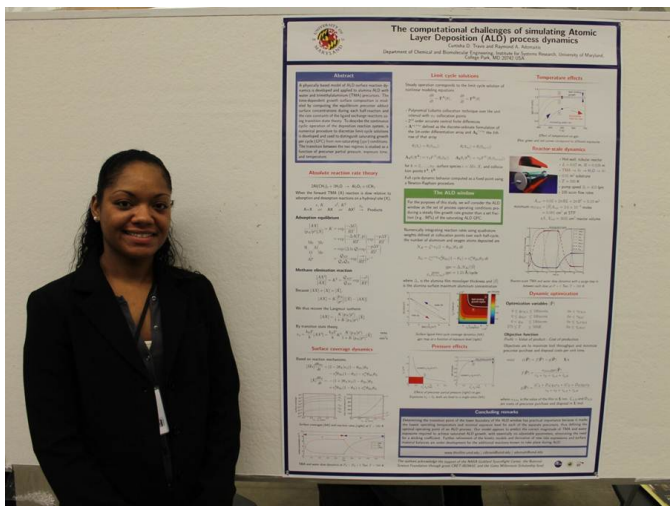
2012 Computing in Chemical Engineering Award Lecture

by Stratos Pistikopoulos

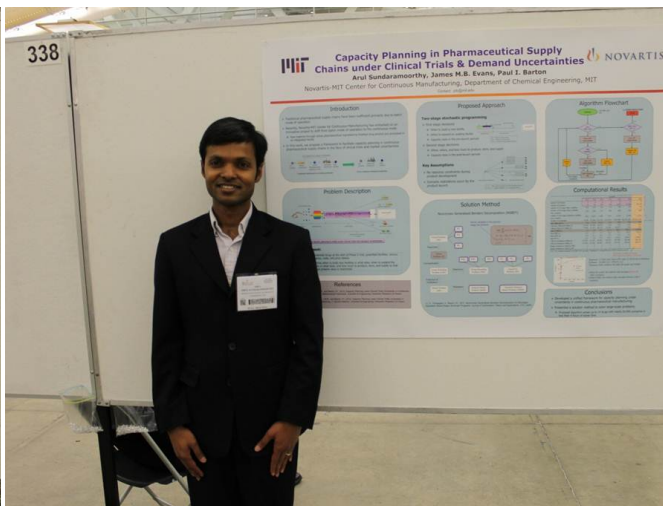
The award lecture, given at the 2012 CAST Awards Dinner in Pittsburgh, PA, is entitled [The Road to Ithaca – Tales in multi-parametric programming and control](#) [3.2MB].



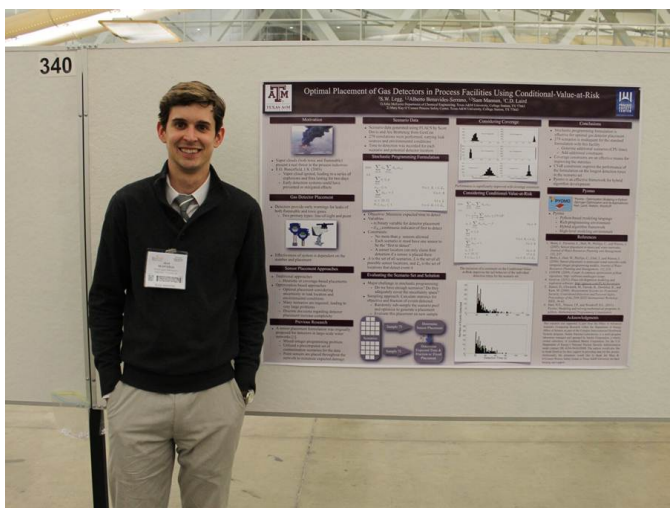
Photos from the 2012 CAST Poster Session and Awards Dinner taken by Marianthi Ierapetritou and Ray Adomaitis



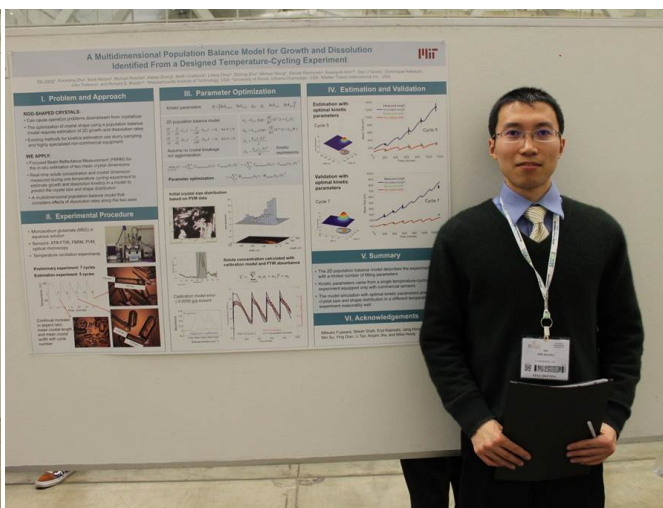
Curtisha D. Travis



Arul Sundaramoorthy



Sean Legg



Mo Jiang



Michael Baldea accepts Cara Toretzky's Award



Richard and Yoshiaki (accompanied by Marianthi on the piano)



Richard, David, Andrew



... and Chris



..., John, and John



... and Stratos



Thank you, Richard!



Some 2012 Travel Grant Winners - Fani, Michael, and Curtisha



CAST Award Winners

2012 Student Travel Grants Awarded

by Matt Bassett, CAST Director

I am happy to announce the winners of the 2012 CAST Graduate Travel Awards. Each award winner received \$500 in support of travel expenses to present one or more papers at the Annual AIChE meeting. Additionally, each awardee received a complimentary ticket to the CAST banquet. The 2013 winners will be announced very soon. The five award winners are:

- **Fani Boukouvala**, Rutgers
Paper 463g
Advisor: Marianthi Ierapetritou
- **Cara Touretzky**, UT Austin
Paper 687b
Advisor: Michael Baldea
- **Michael Nayhouse**, UCLA
Paper 362c
Advisor: Panagiotis Christofides
- **Kody Powell**, UT Austin
Paper 293h
Advisor: Tom Edgar
- **Curtisha Travis**, Maryland
Paper 362d
Advisor: Ray Adomaitis

Please join me in congratulating these winners. Nominations are due next August 1st, 2014, for the [2014 grants](#).

Ray Adomaitis
CAST Travel Grant Chair

2012 CAST Directors' Student Presentation Award

by Matt Bassett, CAST Director

Recognizes a student selected from the CAST Travel Grant recipients for an outstanding oral presentation at the AIChE Annual Meeting.

The winner of this second CAST Directors' Student Presentation Award is **Cara Touretzky** of UT Austin. Congratulations! The title of the presentation is "Modeling and Model Predictive Control Strategies for Building Energy Management". ([Abstract](#)) The Award was acknowledged at last year's annual CAST Division dinner.

Cara received a Bachelors of Chemical Engineering, magna cum laude, from the University of Delaware in 2011 with minors in economics, mathematics, and chemistry. She is currently a graduate student at The University of Texas at Austin, where she is working with her advisor Dr. Michael Baldea to investigate new techniques for modeling and control of large-scale systems, with a particular focus on buildings and controlling their energy use. In her spare time, Cara plays the cello and is a member of the Balcones Community Orchestra in Austin.



The judges would like to thank all the submitters and congratulate them on very nice presentations and materials provided. We were very impressed by all of them. This Award is combined with the CAST Travel Grant. The students selected to receive the grant were asked to provide the documents needed, which were then considered for the Student Presentation Award. Many thanks for all your participation. Congratulations!

Announcements

How to Contact AIChE

Publication sales, meeting registration, applications for membership, technical training, and other AIChE products and services may be obtained by visiting [AIChE Contacts](#).

For answers to specific questions, try one of the [AIChE Staff](#) or one the [CAST Executive Committee](#).


CAST10 E-Mail List

The following website allows anyone to participate in the list:

- listserv.umd.edu/archives/cast10.html is the link that subscribers can use to read and post emails.

The address to post messages to the list is *CAST10 at LISTSERV.UMD.EDU*.

CAST Award Nomination Form

 Please use the [Award Nomination Form](#) [52KB, MS Word], which should be completed by April 15. See [CAST Division Awards](#) for submission guidelines. Electronic submissions are required.

Quote of the Day

There are as many worlds as there are kinds of days, and as an opal changes its colors and its fire to match the nature of a day, so do I.
--- John Steinbeck, *Travels with Charley, in Search of America*

Just as Steinbeck changed his colors and moved on to a new day, so do we, the Editors of this newsletter.

CAST Communications Advertising Policy

Advertising Rates:	1/4 page = \$60; 1/3 page = \$70; 1/2 page = \$90; 2/3 page = \$120; 1 page (8.5" x 11") = \$150
Production Details:	Retain your original art, please. Submit an e-mail containing a WORD or PDF version (contact editor for preferred formats) of your advertisement, to the interim CAST newsletter editor: Karl D. Schnelle .
Deadlines:	December 1 for the Winter issue; July 1 for the Summer issue.
Payment Details:	Prior to publication of advertisement, please submit check payable to CAST Division, AIChE to the CAST Division Secretary/Treasurer
Questions:	Karl D. Schnelle

Join the CAST Division of AIChE

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, which include 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 membership 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](#).

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