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## CAST Communications - Winter 2011-12

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### Editorial Notes

by Peter Rony and Karl Schnelle

Welcome to the Winter 2011 issue of *CAST Communications*. Sometime last year, we learned that approximately 15% of the CAST Division members attend the Fall Annual AIChE meeting. This figure of 15% is true for the other AIChE Divisions, as well. Therefore, it is with great pride and enthusiasm that the Editors present you with this Fall 2011 issue, a truly historic issue of *CAST Communications*. This online newsletter is an important value-added benefit of being a member of the Division.

First, we wish to congratulate our new members of the CAST Division Executive Committee: Professor Marianthi G. Ierapetritou, our Second Vice-Chair; and both Professor Christos T. Maravelias and Dr. John P. Congalidis, who are the 2012-2014 CAST Directors.

Second, we honor the winner of the Directors' Award for the Best Poster at the 2011 AIChE Annual Meeting - Janna Martinek, *et al* - and the honorable mention awardees - Yijie Gao and Fani Boukova, *et al*. Please take the time to click on the links and view the PDF files of their impressive posters.

CAST Division *Award-Lecture-Introducer-Extraordinaire* Wayne Bequette has outdone himself with his introduction to our 2011 Computing-in-Chemical-Engineering Award winner Paul I. Barton. Wayne has provided, for posterity, the photos and dates of our 34 award winners. Please focus your attention on this outstanding group of chemical engineering scholars. To help you with this task, your homework is to match photos with winners. There are 33 awardee names and only 30 photos.

As is tradition, we present the complete award lecture by honoree, Paul I. Barton on Energy Systems Engineering.

In addition, this issue contains several other important announcements. For example, CAST Student Travel Grants were given to five, very deserving students for the Annual AIChE Meeting. This is now the fifth year for these grants. Also, photos of the 2011 CAST poster session and awards dinners are included in this issue. Please have a look below!

Your Editor has been with *CAST Communications* since 1986. During these 25 years, the Editors have made several transitions - from (a) a newsletter that summarized CAST Division session titles, to (b) a printed newsletter that provided articles, communications, and announcements, and finally (c) an online newsletter that included PDF files of session presentations, articles, poster presentations, award lecture introductions, and award presentations at the CAST Division dinner in November. During these 25 years we have succeeded in eliminating the expense associated with printing and mailing the newsletter from the AIChE New York office and also injecting wonderful color images into the newsletter. The Editor thanks the Associate Editor, Karl Schnelle, for his skillful work as producer of the online newsletter. Along the way, the newsletter has won several Max Isaacs awards for outstanding AIChE Division newsletter.

And the [Quote of the Day](#) is by Dom Pérignon.

### Articles


NOTE: The following presentations were given at the CAST Plenary Session at the [2011](#) Annual Meeting of AIChE in Minneapolis, MN.

## Multiscale Modeling and Control of Thin Film Surface Morphology and Microstructure

by Jianqiao Huang, Xinyu Zhang, Gangshi Hu, Gerassimos Orkoulas, and Panagiotis D. Christodes

This work focuses on modeling and control of aggregate thin film surface morphology for improved light trapping using a patterned deposition rate profile. The dynamics of the evolution of the thin film surface height profile are modeled by an Edwards-Wilkinson-type equation (a second-order stochastic partial differential equation) in two spatial dimensions. The thin film surface morphology is characterized in terms of aggregate surface roughness and surface slope. These variables are computed with respect to appropriate visible light-relevant characteristic length scales and defined as the root-mean-squares of height deviation and slope of aggregate surface height profiles, respectively.

Analytical solutions of the expected aggregate surface roughness and surface slope are obtained by solving the Edwards-Wilkinson equation and are used in the controller design. The model parameters of the Edwards-Wilkinson equation can be estimated from kinetic Monte-Carlo simulations using a novel parameter estimation procedure. This parameter dependence on the deposition rate is used in the formulation of the predictive controller to predict the influence of the control action on the surface roughness and slope at the end of the growth process. The cost function of the controller involves penalties on both aggregate surface roughness and mean slope from set-point values as well as constraints on the magnitude and rate of change of the control action. The controller is applied to the two-dimensional Edwards-Wilkinson equation. Simulation results show that the proposed controller successfully regulates aggregate surface roughness and slope to set-point values at the end of the deposition that yield desired levels of thin film reflectance and transmittance levels.

The full presentation is in [pdf](#) [2.4MB ] format.

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## Computer Aided Solvent Selection and Design Framework

by Igor Mitrofanov, Elisa Conte, Gürkan Sin, and Rafiqul Gani

Solvents are widely used as a reaction medium, as a reactant or as carrier at some stages of the manufacturing chain in products from the chemical, fine chemical, pharmaceutical, food, and agrochemical industries. Solvent are either required for processing after which they are removed or they are part of the final product formulation. Therefore, solvents are playing an important role in product synthesis and formulation, product delivery, separation processes etc [1]. On the other hand, solvent selection and design is a complex problem, which requires decision making in several levels for identifying the best candidates depending on different multi-objective criteria namely environment, health, safety, process feasibility and economics.

One of the criteria of solvent selection is the environmental impact because of the excessive consumption and utilization in a wide range of industries, millions of tons solvents have to be wasted every year [2]. Therefore, it becomes important to minimize and optimize the use of organic solvents as much as possible, to satisfy the "Green Chemistry Principles" [3]. Another challenge is that currently solvent selection relies very much on previous experiences, trial and error with different solvent candidates. Such heuristic approach while valuable on their own, however arguably are not fit to deal with a complex multi-criteria optimization and search problem, which is the case for solvent selection.

Therefore the purpose of this contribution is to develop a systematic framework and implement it as software for selection and design of solvents for many applications including organic synthesis, complex reaction systems and solvent-based separations. The solvent selection framework is based on a combination of knowledge from industrial practice and computer-aided tools and methods for property prediction and computer-aided molecular design (CAMD) principles. This framework is applicable for solvent selection and design in product design as well as process design.

The full presentation is in [pdf](#) [1.3MB ] format.

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## Communications

### CAST Election Results

by Karl Schnelle, CAST Secretary

The CAST elections committee is pleased to announce the results of the election of officers for 2012.

Please join us in congratulating our new Second Vice-Chair and two new Directors. Two Directors are elected per year to serve a two year term.



### SECOND VICE-CHAIR: Marianthi G. Ierapetritou

Marianthi Ierapetritou is a Professor in the Department of Chemical and Biochemical Engineering at Rutgers University in Piscataway, New Jersey. She obtained her BS from National Technical University in Athens, Greece, her PhD from Imperial College (London, UK) in 1995 and subsequently completed post-doctoral research at Princeton University (Princeton, NJ) before joining Rutgers University in 1998. Among her accomplishments is the Rutgers Board of Trustees Research Fellowship for Scholarly Excellence that recognizes faculty members who have recently been promoted to associate professor with tenure and whose work shows exceptional promise, and the prestigious NSF CAREER award.

Marianthi's research focuses on the following areas: 1) Process operations; 2) design and synthesis of flexible manufacturing systems; 3) modeling of reactive flow processes; and 4) metabolic engineering. She has published 117 papers and presented in national and international conferences (125 presentations). She was invited to present her work in a number of universities and conferences around the world (44 invitations). She is also a member of INFORMS and SIAM and she active participant in the scientific advisor committees of ESCAPE 16, 17, 21 and PSE 2006, 2009, and FOCAPD 2009. In 2008 she organized the fifth international FOCAPD conference. She is an active educator both in the classroom teaching graduate and undergraduate classes in the Chemical Engineering department and as an advisor currently

supervising the Ph.D. of 9 students and 1 postdoctoral fellow. Her research work is supported by federal (NSF, ONR, PRF, EPA, NIH) and industrial support (Pfizer, ExxonMobil, BOC).

Marianthi has been active in CAST as a program director for the last two years. In this role she initiated an enhancement of the Student travel award to include the Student presentation award which was implemented this year. She has also been a chair for the area 10A programming in 2006 and is an elected Trustee of CACHE for the last 6 years.



#### 2012-2014 DIRECTOR: Christos T. Maravelias

Christos Maravelias was born in 1973 in Athens, Greece. He obtained his Diploma in Chemical Engineering at the National Technical University of Athens in 1996. Next, he moved to the London School of Economics (London, UK), where he received an MSc in Operations Research in 1997. After completing his military service in 1999, he went to Carnegie Mellon University where in 2004 he obtained his PhD in Chemical Engineering. In the fall of 2004 he joined the faculty of the Department of Chemical and Biological Engineering at the University of Wisconsin - Madison. He is a recipient of the Inaugural Olaf A. Hougen Fellowship (University of Wisconsin), an NSF CAREER award, as well as the 2008 W. David Smith Jr. Award from the CAST division of AIChE. Christos' research interests lie in the areas of a) chemical production planning and scheduling; b) supply chain optimization, c) chemical process synthesis, and d) technology assessment for renewable energy.

Christos has been active in CAST programming. He has chaired multiple sessions at the AIChE annual meetings since 2005, and he served as the Area 10C Program Coordinator in 2010. He has also been a member of the FOCAP0 2008, FOCAPD 2009, and PSE 2009 Scientific Committees, and he is currently in the Advisory Committee of FOCAP0/CPC 2012 and PSE 2012.



#### 2011-2014 DIRECTOR: John P. Congalidis

John P. Congalidis is a Research Planning Fellow with DuPont Central Research and Development. His career with DuPont included assignments in advanced process control systems implementation, polymer products development and manufacturing, kinetic modeling, and research management. He has published several refereed journal articles and book chapters in the area of polymerization reactor modeling and control. His contributions to DuPont resulted in three Engineering Excellence Awards. He was the 2010 AIChE Annual Meeting Program Chair for Systems and Control. He received his Diploma in Chemical Engineering from the National Technical University of Athens and his Doctorate in Chemical Engineering from MIT.

#### 2011 CAST Directors' Award


By Martha Grover

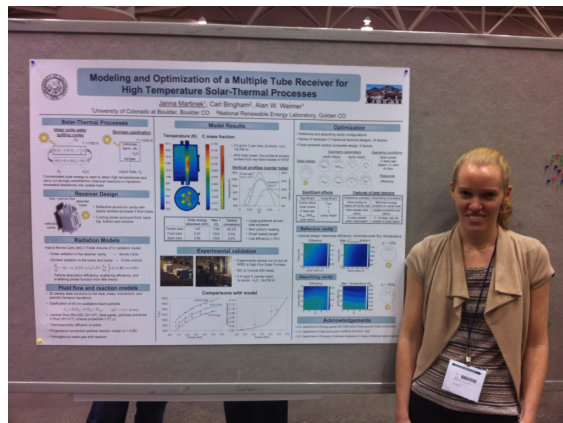
*Given for the best poster presentations at the AIChE Annual Meeting.*

It is my pleasure to announce the winner of the Directors' Award for the Best Poster at the 2011 AIChE Annual Meeting.

The winner of the Directors' Award is:

**First Place:** "Modeling and Optimization of a Multiple Tube Solar Receiver for High Temperature Solar-Thermal Processes.", **Janna Martinek<sup>1</sup>** (with Carl Bingham<sup>2</sup> and Alan W. Weimer<sup>1</sup>), (1)Department of Chemical and Biological Engineering, University of Colorado, Boulder, CO, (2)National Renewable Energy Laboratory, Golden, CO. [Abstract](#).

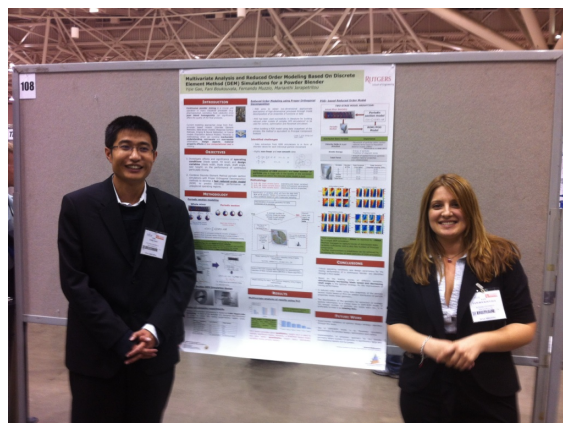
Click on the [photo](#) [644KB 



One honorable mention was also given:

**Honorable Mention:** "Multivariate Analysis and Reduced Order Modeling Based On Discrete Element Method (DEM) Simulations for a Powder Blender", **Yijie Gao and Fani Boukouvala** (with Fernando J. Muzzio and Marianthi G. Ierapertitrou), Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ. [Abstract](#).

Click on the [photo](#) [2.3MB 



## 2011 CAST Award Winners

by Mayuresh V. Kothare, 2010 CAST Second Vice-Chair

### COMPUTING IN CHEMICAL ENGINEERING AWARD



Paul Barton is the Lamot du Pont Professor of Chemical Engineering and Director of the Process Systems Engineering Laboratory at MIT, where he has been since 1992. He received his Ph.D. from the Centre for Process Systems Engineering at Imperial College, London University in 1992. He has held Visiting Professor appointments at CNRS-ENSIC, Nancy, France and EPFL, Lausanne, Switzerland. He has industrial experience with BP and Air Products, and has consulted for major corporations including Dow Chemical, Alstom Power and Aspen Technology. He was awarded the Outstanding Young Researcher Award by AIChE's CAST Division in 2004, and the Indo-American Frontiers of Engineering Award in 2008. Barton's research interests include hybrid discrete/continuous dynamic systems; numerical analysis of ordinary differential, differential-algebraic and partial differential-algebraic equations; sensitivity analysis and automatic differentiation; global, mixed-integer and dynamic optimization theory and algorithms; and open process modeling software. Some of the applications his group is currently focusing on include energy systems engineering, continuous pharmaceutical manufacturing and nano-scale systems engineering. He served as Director for AIChE's CAST Division from 2001-2004 and is currently a subject editor for Optimal Control Applications and Methods and associate editor for Journal of Global Optimization and Journal of Optimization Theory and Applications. He is author or co-author of over 100 articles in refereed journals. He has been very active in the design and the development of process modeling software, having been the original author of gPROMS, and having led the development of ABACUSS/JACOBIAN and DAEPACK at MIT, all of which are now commercial products widely used in industry.

### COMPUTING PRACTICE AWARD



Don Bartusiak is R&D Program Lead for process control at ExxonMobil Research & Engineering. He has 23 years of experience with ExxonMobil in technical and supervisory positions in the U.S. and Europe covering regulatory control, linear and nonlinear MPC, realtime optimization, and online artificial intelligence technologies for businesses ranging from refining to petrochemicals. He was Lecturer and Adjunct Professor of Chemical Engineering at Rice University from 2000 to 2001. From 1977 to 1984, he was a process development research engineer Bethlehem Steel Corporation. He has a B.S. degree from the University of Pennsylvania, and M.S. and Ph.D. degrees from Lehigh University. Don is co-author of 16 technical articles, and co-inventor on 3 U.S. patents and multiple international patents. He is currently co-chair of the CPC VIII conference. He is a past Director of the CAST Division, and past chairman of the Process Control programming committee of the Ethylene Producers Conference. He held multiple offices in the AIChE Lehigh Valley Section, including Section Chairman in 1982.

### OUTSTANDING YOUNG RESEARCHER AWARD



Martha Grover is an Associate Professor in the School of Chemical & Biomolecular Engineering at the Georgia Institute of Technology. She earned her BS from the University of Illinois, Urbana-Champaign, and her MS and PhD from the California Institute of Technology. She joined Georgia Tech as an Assistant Professor in 2003, and received an NSF CAREER award in 2004. Her research program is dedicated to understanding, modeling, and engineering the self-assembly of atoms and small molecules to create larger scale structures and complex functionality. Her approach draws on process systems engineering, combining modeling and experiments in applications including surface deposition, fluid-phase crystallization, polymer reaction engineering, and neural cultures. She is a member of the NSF Center for Chemical Evolution and the Georgia Tech Center for Organic Photonics and Electronics.

### DAVID HIMMELBLAU AWARD



Dr. Francis J. Doyle III is the Associate Dean for Research in the College of Engineering at UC, Santa Barbara and he is the Director of the Army Institute for Collaborative Biotechnologies. He holds the Duncan and Suzanne Mellichamp Chair in Process Control in the Department of Chemical Engineering, as well as appointments in the Electrical Engineering Department, and the Biomolecular Science and Engineering Program. He is the recipient of several research awards (including the NSF National Young Investigator, ONR Young Investigator, Humboldt Research Fellowship) as well as teaching awards (including the Purdue Potter Award, the ASEE Ray Fahien Award, and the ASEE Chemstations Lectureship Award). He is a Fellow of multiple professional societies including IEEE, IFAC, AIMBE, and AAAS. In 2005, he was awarded the Computing in Chemical Engineering Award from the American Institute of Chemical Engineers for his innovative work in systems biology. His research interests are in systems biology, network science, modeling and analysis of circadian rhythms, drug delivery for diabetes, model-based control, and control of particulate processes.



Ed Gatzke is currently an Associate Professor in the Department of Chemical Engineering at the University of South Carolina. He received his undergraduate degree from Georgia Tech in 1995 and his PhD degree from the University of Delaware in 2000. His awards include the NSF Career Award, the USC CEC Young Investigator Award, the Alexander von Humboldt Experienced Researcher Fellowship, and the USC Mortar Board Excellence in Teaching Award. Ed currently lives in Columbia, SC with his wife Andi and their two children, Drew and Ellie.



Robert S. Parker is an Associate Professor in the Department of Chemical and Petroleum Engineering at the University of Pittsburg his BS from the University of Rochester in 1994 and his PhD from the University of Delaware in 1999, both in Chemical Engineering. He is also a member of the University of Pittsburgh Cancer Institute, the McGowan Institute for Regenerative Medicine, and serves as the faculty advisor to Order of the Engineer Link #23. Prof. Parker won the NSF CAREER Award in 2002 and the Carnegie Science Center Award for Excellence in Higher Education in 2008 for the Pitt Pillars Curriculum. The Parker lab works primarily in the area of systems medicine - the integration of systems engineering and biology/medicine to aid the human condition - with disease foci in cancer chemotherapy, diabetes, and inflammation.

### DAVE SMITH JR. GRADUATE PUBLICATION AWARD



Fengqi You received his PhD from Carnegie Mellon University in 2009 and a BS from Tsinghua University in 2005, both in chemical engineering. His graduate research with Professor Ignacio Grossmann is concerned with the development of mixed-integer nonlinear programming models and algorithms for the design and operations of chemical processes and supply chains under uncertainty. From 2009 to 2011, he was an Argonne Scholar at Argonne National Laboratory, where his efforts were concentrated on the analysis, design and optimization of sustainable energy systems. He started as an Assistant Professor of Chemical and Biological Engineering at Northwestern University in 2011. The research of his group focuses on the development of novel computational models, optimization techniques and systems analysis methods for problems in process-energy-environmental systems engineering. Fengqi has published over 25 journal articles and book chapters. His recent honors include the Director's Postdoctoral Fellowship from Argonne National Laboratory (2009-2011) and the Ken Meyer Award for best doctoral thesis in chemical engineering at Carnegie Mellon University (2010).

### Award Lecture Introduction

by B. Wayne Bequette, 2006 CAST Chair

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

Wayne presented an [introduction](#) [2.3MB ] to the attendees of the 2011 CAST Awards Dinner.



[cbe.rpi.edu]

### 2011 Computing in Chemical Engineering Award Lecture

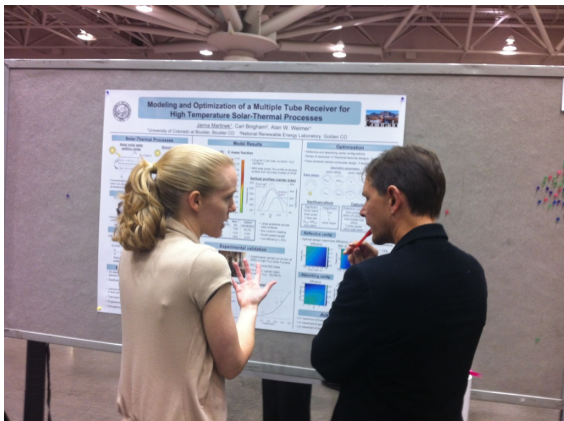
by Paul I. Barton

The award lecture, given at the 2011 CAST Awards Dinner in Minneapolis, MN, is entitled [CAST Computing in Chemical Engineering Award Talk](#) with emphasis on Energy Systems Engineering [[11MB](#) ].

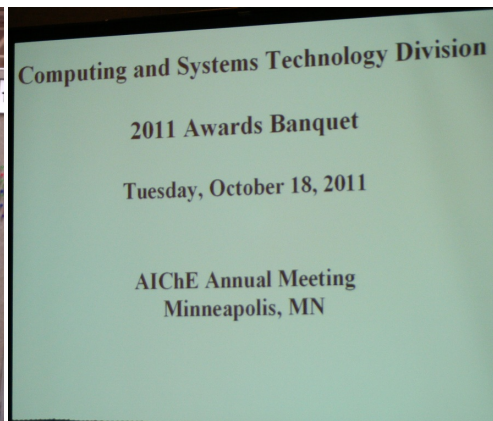


### Photos from the 2011 CAST Poster Session and Awards Dinner

taken by Tom Badgwell, Matt Bassett, and Mayuresh Kothare



Intense discussion at the poster session



What, when, and where



Don receives his award



Fengqi after receiving his award



Martha and her award



Frank, Ed, & Robert receive their award



Thank you, Mahmoud!



Wayne's intro to Paul



yada yada yada...



Paul receives the Computing Award



Paul giving his talk

## 2011 Student Travel Grants Awarded

by Ray Adomaitis

I am happy to announce the winners of the 2011 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 five award winners are:

- **Hector Galicia**, Auburn University: Fault Detection and Diagnosis in the Statistics Pattern Analysis Framework  
Paper 404b, Process Monitoring, Fault Detection, and Diagnosis I  
Advisor: Jin Wang
- **Carlos Henao**, University of Wisconsin: A Modeling Approach for Chemical Process Synthesis  
Paper 330E, Process Design II  
Advisor: Christos Maravelias
- **Juan Du**, Carnegie Mellon University: Stability Condition and Discretization Scheme for the Population Balance  
Paper 646f, Dynamics, Reduction and Control of Distributed Parameter Systems  
Advisor: Erik Ydstie
- **Siam Aumi**, McMaster University: Adaptive Data-Based Model Predictive Control of Batch Systems  
Paper 669b, Process Modeling and Identification  
Advisor: Prashant Mhaskar
- **Xiaoxiang Zhu**, MIT: Mathematical Modeling of Intravascular Drug Delivery In Drug-Eluting Stents with Biodegradable Coating  
Poster 621e, Poster Session Applied Mathematics and Numerical Analysis  
Advisor: Richard Braatz

Please join me in congratulating this year's winners. Nominations are due August 1st for the [2012 grants](#).

Ray Adomaitis  
CAST Travel Grant Chair

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### 2011 CAST Directors' Student Presentation Award

by Marianthi Ierapetritou, for the CAST Directors

To recognize a student for an oral presentation delivered at the AIChE Annual Meeting starting this year, CAST recently established the CAST Director's Student Presentation Award. The winner of this first CAST Presentation Award is **Hector Galicia** of Auburn University. Congratulations! The Award will be acknowledged in next year's annual CAST Division dinner.

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 year this Award was combined with the CAST Travel Grant. The students selected to receive the grant were asked to provide the documents needed and then considered for the Presentation Award. Many thanks for all your participation. Congratulations!

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## 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](#) or using the [On-line contact form](#).

For answers to specific questions, try one of the following [AIChE Staff](#):

<a href="#">Felicia Guglielmi</a> Director, Volunteer and Membership Activities	<a href="#">Bette Lawler</a> Director, Operations
<a href="#">Joseph Cramer</a> Director, Technical Programming	<a href="#">Steve Smith</a> Director, Technical Activities and Publications


### CAST10 E-Mail List

The following websites are used to participate in the list:

1. [listserv.umd.edu/archives/cast10.html](http://listserv.umd.edu/archives/cast10.html) is the link that subscribers can use to read and post emails.
2. [www.ench.umd.edu/cast10/](http://www.ench.umd.edu/cast10/) has lots of older emails.

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

### 2012 Award Nomination Form

 Please use the [2010 Award Nomination Form](#) [52KB, MS Word], which should be completed by April 15, 2012. See [CAST Division Awards](#) for submission guidelines. Electronic submissions are required.

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### Quote of the Day

*Come quickly, I am drinking the stars!* --- Dom Pérignon

Dom Pérignon may get all the credit for Champagne, but wiki says it was actually an English scientist and glass maker, Christopher Merret, who published a paper in 1662 concerning secondary fermentation to produce the bubbles. Have a great New Years!!!

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### CAST Communications Advertising Policy

<b>Advertising Rates:</b>	1/4 page = \$60; 1/3 page = \$70; 1/2 page = \$90; 2/3 page = \$120; 1 page (8.5" x 11") = \$150
<b>Production Details:</b>	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 CAST newsletter editor: <a href="#">Peter R. Rony</a> .
<b>Deadlines:</b>	December 1 for the Winter issue; July 1 for the Summer issue.
<b>Payment Details:</b>	Prior to publication of advertisement, please submit check payable to CAST Division, AIChE to the <a href="#">CAST Division Secretary/Treasurer</a>
<b>Questions:</b>	<a href="#">Peter R. Rony</a> , Telephone (540) 951-2805

## 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 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](#).

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Associate Editor: Karl D. Schnelle, Dow AgroSciences LLC