

**CAPD e-Newsletter, October 2007**

<http://capd.cheme.cmu.edu>

Dear CAPD member,

Welcome to the CAPD e-Newsletter!

We hope this newsletter will have information that is of interest to you.

Best regards, Ignacio Grossmann

- We continue to grieve the unexpected death of our colleague, Professor Gary Powers who we sorely miss. There was a memorial service at the university on September 13 that was well attended. Also, Dr. Jeff Sirola gave a talk on October 3 where he described the collaboration he had with Gary at Wisconsin during their Ph.D. studies, and which led to the invention of the concept of process synthesis. In his memory an undergraduate scholarship has been established. Donations may be sent for the Gary J. Powers Scholarship Fund, c/o Toni McIltrout, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213-3890.

- The CAPD webpage has been updated by Heather Widmayer and has a totally new look. Please visit the webpage at: <http://capd.cheme.cmu.edu> and let us know if you have any comments.

- Please take note that the next Annual Review Meeting will take place on March 10-11, 2008. This will be followed by the meeting of the special group on Enterprise-wide Optimization on March 12.

- New CAPD Short course: <http://capd.cheme.cmu.edu/shortcourse/index.html>  
The CAPD short course next year will take place on June 12-18, 2008. With the addition of Nick Sahinidis to CAPD, the course has been reorganized. Also, Erik Ydstie will be participating.

The new course Optimization Modeling and Integrated Process Operations is organized in two modules:

I. Optimization Modeling to be taught from Thursday through Saturday (June 12-15) will focus on modeling and algorithms with applications to process optimization, process synthesis and molecular design:

- a) Nonlinear programming (Biegler, Thursday, June 12)
- b) Mixed integer and disjunctive programming (Grossmann, Friday, June 13)
- c) Global optimization and optimization under uncertainty (Sahinidis, Saturday, June 14)

II. Integrated Process Operations to be taught from Monday through Wednesday (June 16-18) will focus on three major decision levels in plant and enterprise-wide optimization:

- d) Mixed-integer models for planning and scheduling (Grossmann, Monday, June 16)
- e) Process dynamics and control (Ydstie, Tuesday, June 17)
- f) Differential/algebraic models for real time optimization (Biegler, Wednesday, June 18)

The material in each module is independent and self-contained and can be taken in any combination. A detailed description of the topics covered in the course is given in: [http://capd.cheme.cmu.edu/shortcourse/shortcourse\\_details.htm](http://capd.cheme.cmu.edu/shortcourse/shortcourse_details.htm). Recall that CAPD members receive a 25% discount.

- Pan American Advanced Study Institute on Emerging Trends In PSE.

Ignacio Grossmann will be organizing with Frank Doyle, Jaime Cerda and Argimiro Secchi the Pan American Advanced Studies Institute (PASI) on emerging trends in Process Systems Engineering on August 12-21, 2008, in Hotel Costa Galana, Mar del Plata, Argentina. The proposed workshop is aimed at advanced graduate and post-doctoral students, and will emphasize the latest developments and research challenges in the emerging areas of sustainability, energy, biological systems, multiscale systems, and enterprise-wide optimization. The PASI workshop will be a follow-up to the successful PASI on Process Systems Engineering that took place on in Iguazú, Argentina, in 2005.

We also plan to produce a virtual library as we did in the previous meeting, and therefore would greatly appreciate financial support to supplement the funding by NSF.

Information about this meeting can be found in: <http://cepac.cheme.cmu.edu/pasi2008/>

- Enterprise-wide Optimization <http://egon.cheme.cmu.edu/ewocp/>

TOTAL has joined the EWO group which has been composed by ABB, Air Products, BP, Dow Chemical, ExxonMobil and NOVA Chemicals. The next meeting of the EWO will take place on Tuesday, November 13. The meeting will feature presentations by industrial participants and shorter reports by students and faculty.

Companies interested in participating in this research program should contact [grossmann@cmu.edu](mailto:grossmann@cmu.edu)

- Special Issue on Enterprise-wide Optimization (EWO) in *Computers & Chemical Engineering*. Kevin Furman and Ignacio Grossmann are completing the editing of this special issue. We expect the issue will appear mid-2008.

- Faculty News

- As we announced in our last newsletter, Nick Sahinidis has joined our department and is in the CAPD. Nick gave the Applied Mathematics Colloquium "Global optimization with branch-and-reduce" in the Department of Mathematics at the Massachusetts Institute of Technology on October 1, 2007

- Ignacio Grossmann received the degree of Doctor Honoris Causa from the University of Maribor in Slovenia. He was cited for his work on MINLP and synthesis and flexibility for process systems.

- Larry Biegler and Erik Ydstie will be recognized at the AIChE Meeting in Salt Lake City. Larry for obtaining the 2007 CACHE Award for Excellence in Computing in Chemical Engineering Education, and Erik for receiving the 2007 AIChE Computing in Chemical Engineering CAST Award.

- Ignacio Grossmann delivered the keynote lecture, "Computational Methods for Enterprise-wide Optimization of Process Industries," at the Workshop on Supply Chain Optimization, Institute of Chemical Engineering Sciences, Singapore, August (2007). He also delivered the plenary lecture, "Optimal Design of Process Systems with Renewable Resources," at the 1st International Symposium on Sustainable Chemical Product and Process Engineering, Guangzhou, China (2007).

- Erik Ydstie delivered the plenary lecture "Optimality of Integrated Process and Financial Networks", at the international conference on Integrated Operations in Trondheim, Norway on October 1. This conference focuses on the problem of how to integrate large subsea oil and gas-field management with markets in real time. He also was part of a panel discussion on energy as part of the Keenan symposium on "Meeting the Entropy Challenge" in the Department of Mechanical Engineering at MIT. The meeting boasted the participation of Nobel prize in physics and economics. One major conclusion appeared to emerge: The Maxwell Demon is dead. Erik is presenting seminars at Notre Dame University in October and at US Davies in December. He is currently on leave to write a new undergraduate textbook on process control and he is also running ILS Inc as CEO of the start-up company. He delivered a plenary lecture called "Dissipation and Invariance in Process Networks" at the Model Reduction workshop at the University of Leicester in the UK in August.

- Student News

- Congratulations to Muge Erdirik-Dogan and Ramkumar Karuppiah for successfully defending their Ph.D. thesis early in September. Muge has joined Amazon, while Ram will be joining Dow Chemical.

- Congratulations to Gaurav Bansal for successfully completing his M.S. thesis early in September. Gaurav will be joining Bayer Corporation.

- Congratulations to Bora Tarhan for receiving honorable mention at the CHEGSA meeting for his talk "Oilfield Exploration and Production Operations under Uncertainty." Congratulations also to Juan Ruiz who received the Gary Powers Award for Best Poster Presentation for his work "Global Optimization of Bilinear Generalized Disjunctive Programs." Both Bora and Juan are working with Ignacio.

- Congratulations to Alexander Smith who was selected to receive a travel grant from CAST in conjunction with the AIChE meeting in Salt Lake City.

- Congratulations to Parag Jain for completing his Ph.D. proposal

- The following PSE students successfully passed their Ph.D. qualifying exam:  
Rui Huang, Weijie Lin and Sree Rama Raju Vetukuri, working for Larry Biegler  
Abdulrahman Alattas, Ravi Kamath , Sylvain Mouret and Juan Ruiz, working for Ignacio Grossmann. Michael Wartmann, working for Erik Ydstie.

-Webpages. The following sites might be of interest to you:

Virtual library on Process Systems Engineering:

<http://cepac.cheme.cmu.edu/pasilectures.htm>

You can access webpages of all PSE faculty in the Americas in:

<http://cepac.cheme.cmu.edu/country.htm>

Papers to be presented by CAPD faculty at AIChE Meeting, Salt Lake City:

-Larry Biegler's group:

Effects of Substrate Geometry on the Deposition Process in A Cvd Reactor

Yousef Sharifi, Luke E. K. Achenie, Lorenz T. Biegler

<http://aiche.confex.com/aiche/2007/techprogram/P96300.HTM>

A Moving Horizon Estimation Algorithm Based on Nlp Sensitivity

Victor M. Zavala and Lorenz T. Biegler

<http://aiche.confex.com/aiche/2007/techprogram/P84195.HTM>

Modeling and Optimization of Polymer Electrolyte Membrane Fuel Cells

Parag Jain, Lorenz T. Biegler, and Myung S. Jhon

<http://aiche.confex.com/aiche/2007/techprogram/P90337.HTM>

Stability and Performance Analysis of Nlp Sensitivity-Based Nmpc Controllers

Victor M. Zavala and Lorenz T. Biegler

<http://aiche.confex.com/aiche/2007/techprogram/P84191.HTM>

Modeling of Polymer Electrolyte Membrane and Proton Transport via Atomic Scale  
Molecular Dynamics Simulation

Pil Seung Chung, Parag Jain, Haigang Chen, Lorenz T. Biegler, and Myung S. Jhon

<http://aiche.confex.com/aiche/2007/techprogram/P95559.HTM>

Lbm Flow Simulation in the Porous Media Using Representative Elementary Volume  
Method

Pil Seung Chung, Parag Jain, Hyung Min Kim, Lorenz T. Biegler, and Myung S. Jhon  
<http://aiche.confex.com/aiche/2007/techprogram/P95615.HTM>

Reduced-Order Model for Dynamic Optimization of Pressure Swing Adsorption  
Anshul Agarwal, Lorenz T. Biegler, and Stephen E. Zitney  
<http://aiche.confex.com/aiche/2007/techprogram/P84361.HTM>

A Brief Chronology of Process Optimization  
Lorenz T. Biegler  
<http://aiche.confex.com/aiche/2007/techprogram/P99687.HTM>

Advanced Process Engineering Co-Simulation Using Cfd-Based Reduced Order Models  
Yi-dong Lang, Lorenz T. Biegler, Sorin Munteanu, Jens Madsen, and Stephen E. Zitney  
<http://aiche.confex.com/aiche/2007/techprogram/P88963.HTM>

Efficient Parallel Solution of Dae Constrained Optimization Problems with Loosely Coupled Algebraic Components  
Carl D. Laird, Victor M. Zavala, and Lorenz T. Biegler  
<http://aiche.confex.com/aiche/2007/techprogram/P95091.HTM>

-Ignacio Grossmann's group

Optimal Synthesis of Para-Xylene Separation Processes Based on Crystallization  
Ricardo M. Lima and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P83968.HTM>

Decomposition Method for Solving Mixed Integer Nonlinear Model for Oilfield Exploration And Production Operations Under Uncertainty  
Bora Tarhan and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P86135.HTM>

Design of Responsive Supply Chains under Demand Uncertainty  
Fengqi You and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P87597.HTM>

Optimization under Uncertainty for the Design and Planning of Process Systems  
Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P101770.HTM>

Global Optimization of Bilinear Generalized Disjunctive Programs  
Juan P. Ruiz and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P91764.HTM>

A Slot-Based Formulation for Short-Term Scheduling of a Two-Stage Batch Plant with Parallel Reactors with Sequence-Dependent Changeovers

Muge Erdirik-Dogan, Ignacio E. Grossmann and John Wassick  
<http://aiche.confex.com/aiche/2007/techprogram/P88947.HTM>

Optimal Design and Planning of Sustainable Chemical Supply Chains under Uncertainty  
Gonzalo Guillén-Gosálbez and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P86632.HTM>

Batching and Scheduling of Single Stage Batch Plants with Sequence Dependent Changeovers: A Comparative Study  
Pedro Castro, Muge Erdirik-Dogan and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P89554.HTM>

Considering Isothermal Streams in the Minlp Synthesis of Heat Exchanger Networks  
Arturo Jiménez, José M. Ponce, and Ignacio E. Grossmann  
<http://aiche.confex.com/aiche/2007/techprogram/P92669.HTM>

- Nick Sahinidis' group:

A Novel Integer Minimal Principle with Atomicity Constraints for Phasing Single-Crystal X-Ray Diffraction Data  
Alexander B. Smith and Nick Sahinidis.  
<http://aiche.confex.com/aiche/2007/techprogram/P97214.HTM>

Automatic Convexity Detection for Global Optimization  
Xiaowei Bao, Nick Sahinidis  
<http://aiche.confex.com/aiche/2007/techprogram/P97289.HTM>

Erik Ydstie's group:

A New Approach for Adaptive Control and Identification using Selective Memory Supervision  
Eduardo J. Dozal-Mejorada and B. Erik Ydstie  
<http://aiche.confex.com/aiche/2007/techprogram/P97468.HTM>

Complex Dynamics in Decentralized Networks of Adaptive Systems  
Eduardo J. Dozal-Mejorada and B. Erik Ydstie  
<http://aiche.confex.com/aiche/2007/techprogram/P97591.HTM>

Uniqueness and Stability of the Steady State in Flash Reactors  
Yuan Xu, Eric Ydstie  
<http://aiche.confex.com/aiche/2007/techprogram/P97200.HTM>

Modeling for Design and Control of Multi-Phase Reactors  
Mohit Aggarwal, B. Erik Ydstie, and Lee R. White  
<http://aiche.confex.com/aiche/2007/techprogram/P97400.HTM>

From Batch to Cyclic Process: Optimality and Stability

Yuan Xu, Erik Ydstie

<http://aiche.confex.com/aiche/2007/techprogram/P97158.HTM>

New Vistas for Process Control: Integrating Physics and Communication Networks

B. Erik Ydstie

<http://aiche.confex.com/aiche/2007/techprogram/P97475.HTM>

- Upcoming meetings

INFORMS Annual Meeting, November 4-7, 2007

Seattle, WA

<http://meetings.informs.org/Seattle07/>

2007 AIChE Annual Meeting, November 4 -9, 2007

Salt Lake City, Utah

<http://www.aiche.org/Conferences/AnnualMeeting/index.aspx>

5th International Logistics and Supply Chain Congress, November 8-9, 2007-10-21

Istanbul, Turkey

<http://lm-scm2007.okan.edu.tr/>

INFORMS Practice Conference: Applying Science to the Art of Business

April 13-15, 2008

Baltimore, Maryland

2008 AIChE Spring National Meeting, April 6-10, 2008

New Orleans, LA

<http://www.aiche.org/Conferences/SpringMeeting/index.aspx>

SIAM Conference on Optimization (OP08), May 10-13, 2008

Boston, Massachusetts

<http://www.siam.org/meetings/calendar.php?id=191>

Applied Mathematical Programming and Modelling (APMOD 2008), May 28-30, 2008

Bratislava, Slovakia

<http://www.apmod2008.org/>

ESCAPE'18, June 1-4, 2008

Lyon, France

<http://www.escape18.org/>

2008 Process Development Symposium: Chemical Product Engineering - The Third Paradigm, June 22-25, 2008

The Berkshires, Hancock, MA

<http://www.aiche.org/Conferences/Specialty/ProcessDevelopment.aspx>

International Conference on Engineering Optimization, June 1-5, 2008  
Rio de Janeiro  
<http://www.engopt.org/>

2008 FOCAPO Meeting, June 29 - July 2, 2008  
Cambridge, Massachusetts, USA  
<http://www.focapo.org/>

18th Triennial Conference of IFORS, July 14, 2008 - July 18, 2008  
Sandton, South Africa

INFORMS Annual Meeting 2008, October 12-15, 2008  
Washington, DC

2008 AIChE Annual Meeting, November 16-21, 2008  
Philadelphia, PA  
<http://www.aiche.org/Conferences/AnnualMeeting/annual2008.aspx>

2009 PSE'09 , Aug. 16-20, 2009  
Salvador, Brazil  
<http://www.cepema.usp.br/pse2009>

World Congress Chemical Engineering, Aug. 23-29, 2009  
Montreal, Canada  
<http://www.chemengcongress2009.com/>