

THE CHEME NEWS
Internal Newsletter of the Department of Chemical Engineering
Carnegie Mellon University
Spring 2013

Message from the Department Head

As you may know, I am promoting myself back to Full Professor this year; and so, this will quite likely be the last ‘Message from the Department Head’ that I write. No need for concern though; I am sure that an excellent replacement will be in the position by Fall, just in time to write the next ‘Message from the Department Head’. Ignacio Grossmann is chairing the committee to make recommendations to Dean Jim Garrett concerning the next department head and the directions that the department wishes to take. The committee is actively seeking input from all of us, and I would encourage you to express to them any thoughts that you have on the future of the department.

The good news is that because there are so many things going on in the department there is no shortage of material to cover in these newsletters. Perhaps the most obvious and important news of the past semester was the election of Larry Biegler to the National Academy of Engineering. This is a great recognition for Larry and for the Department. In addition, others of our colleagues and students have won awards that you can read about in later sections of this newsletter. Equally importantly, we have two new colleagues Megan Mauter and Katie Whitehead who joined us late last semester and possibly two more who will join us over the summer. And, of course, the other promotion to Full Professor is that of Shelley Anna. Congrats to all!

One of the things that I have come to appreciate as Department Head is that steady state is not a valuable objective when it comes to an organization like CMU and a department like ours. Steady state may be nice from the point of operational simplicity and solving a few problems in chemical engineering, but you cannot write interesting newsletters about departments in steady state. Change is a good thing and momentum is a sign of a healthy organization; otherwise all that you have is inertia. I am sure that collectively we will continue to find ways to improve the department and implement positive changes in our program. If we continue to do it faster and better than the competition, only good things can come.

With those thoughts, I am going to head back to the lab and my still pristine ‘other’ office and from there dive into the trenches to beat back the frontiers of science and engineering.

Andy

Department News

CPS Outreach

Many thanks to the students who volunteered their time at the Carnegie Science Center for National Chemistry Week (NCW) in October and National Engineers Week (NEW) in February. Volunteers for NCW were: Sharon Vuong, Melissa Day, Denise Posluszny, Nicole Asermely, Ben Yezer, John Riley and Stephanie Kirby. NEW volunteers were: Bethany Nicholson, Sharon Vuong, Melissa Dao, Chong Ren, Sarah Feight, Zefan Jiang, Jacob Boes, Lei Wang, Nichole Asermely, Ye Wang, Denise Posluszny, Ben Yezer, Zixiang Gao, Huangquiang Zhao, Jingniang Cheng, Ning Xin, Zilong Wang, and Javier Lanauze. Nearly 4,000 people visited the Science Center for each event and the organizers were very complimentary of our efforts and the content of our displays. Future Summer CPS Outreach events include CIT Scouting for Engineers and the ICES Summer Engineering Experience for Girls. Contact Rosemary Frollini or Annette Jacobson for more information.

Faculty News

Larry Biegler NAE recipient honored at ChemE reception on February 7, 2013



Andy Gellman, Erik Ydstie, Art Westerberg, Larry Biegler, Ignacio Grossmann

Larry Biegler presented a short course entitled Strategies for Nonlinear On-line Optimization in the Department of Systems Engineering and Automation, University of Valladolid, Valladolid, Spain, during the week of September 15-22. An invited talk entitled “Model Reduction for Multi-scale Optimization” was presented at the International Seminar on Production Planning and Scheduling at CENPES/Petrobras, Rio de Janeiro, during October 9-11. Larry participated in

the 1st International Symposium “InPROMPT 2012” sponsored by the Technical University of Berlin, where on November 16th he gave a presentation entitled “Optimization Tools for Process Modeling and Design.” Finally, on January 25, Larry will receive an honorary doctorate in engineering sciences (Dr.-Ing. E.h.) from the Technical University of Berlin. More information on this can be found on: http://www.pressestelle.tuberlin.de/menue/veranstaltungen/veranstaltungen_des_praesidenten/ehrendoktorwuerde_prof_biegler//. In addition, from Jan. 15-18, Larry participated in a DOD Workshop in Austin, TX. On Feb. 21, he presented a seminar entitled “Multi-scale Optimization for Integrated Design of Engineering Systems” at ExxonMobil Corporate research. From March 6-7, Larry participated in a Reduced Order Modeling workshop, sponsored by LBL and NETL and gave a talk entitled “Overview of reduced order modeling techniques: state of the art and challenges.” Finally, Larry was elected as member of the National Academy of Engineering in February, 2013.

Andy Gellman is organizing a symposium on Enantioselective Properties of Chiral Surfaces at the Spring ACS meeting in New Orleans. Later he will be attending a Gordon Conference in Switzerland in April and then giving a keynote lecture at the Meeting of the North American Catalysis Society in June.

Ignacio Grossmann attended the INFORMS Computing Meeting in Santa Fe, NM., January 6-9, 2013, where he presented the papers “Global Optimization of Mixed-Integer Bilinear Programs With a Multiparametric Disaggregation Technique,” and “An Algorithm for Preprocessing and Tightening Generalized Disjunctive Programming Models Through the Application of Basic Steps.” He then went to the Instituto Tecnológico de Celaya where he taught a short course on mixed-integer programming and enterprise-wide optimization. He was also awarded the Agustin Vazquez Vera Lectureship, for which he gave the talk “Optimal Synthesis and Planning of Sustainable Chemical Processes.” He then visited Taiwan where he gave the talk “Challenges in the Application of Mathematical Programming in the Enterprise-wide Optimization of Process Industries” at the National Taiwan University. He also gave the talk “Optimal Synthesis and Planning of Sustainable Chemical Processes” at the PSE Symposium in Hsinchu. In March he gave the seminar “Optimal Synthesis and Planning of Sustainable Chemical Processes” at Drexel University. Next he went to Sweden where he participated in the Process Integration Jubilee in Gothenburg in March 18-20 where he gave the talks, “Recent Developments in the Application of Mathematical Programming to Process Integration” and “Role of Process Integration in Process Systems Engineering.” On April 11, Ignacio was awarded the Inaugural Leslie Shemilt Lectureship at McMaster University in Canada with the talk “Optimal Synthesis and Planning of Sustainable Chemical Processes.” Finally, on April 22, he will give the seminar “Relaxations for Convex Nonlinear Generalized Disjunctive Programs and their Application to Nonconvex Problems,; at Texas Tech University. Finally, Ignacio was appointed chair of the search committee for the Department Head in Chemical Engineering.

Jim Miller has been elected a fellow of the American Institute of Chemical Engineers (AIChE) in recognition of his professional achievements, significant accomplishment in the area of catalysis, and especially for his outstanding leadership and service in the Pittsburgh local section of AIChE. Jim will be recognized at an upcoming Pittsburgh meeting.

Jeff Siirola continues to divide his time between CMU and Purdue and for the Spring Semester was mostly at Purdue, although he did return for the CAPD Annual Review Meeting where he made a short presentation of the history of natural gas production, use, and regulation in the US which ultimately lead to the development of shale gas recovery technology. He also contributed several sessions on process synthesis for the new CMU graduate level process systems modeling course which is being offered for the first time. While at Purdue, Jeff taught the capstone senior process design course and developed new materials that will be useful as he and Ignacio again co-teach a similar course at CMU this next Fall. He also taught and refined a chemical technology and industry structure course based on one first developed at CMU last year and which will also be taught at CMU again this next Fall. Jeff also participated in a workshop on teaching senior design at the AIChE Midwest Regional Conference in Chicago, delivered a keynote on the role of integration in process synthesis at the International Process Integration Jubilee Conference in Gothenburg, delivered departmental seminars on process synthesis at Imperial College and Columbia, and participated in the Carbon Capture Simulation Initiative industrial advisory board workshop. He also participated in engineering outreach at an inner-city elementary school in Los Angeles, departmental advisory board meetings at Georgia Tech, Tennessee Tech, South Carolina, and the University of Delaware Energy Institute, and continued his service as ABET Secretary.

Nick Sahinidis. In October, he attended the Industrial Advisory Board meeting of the Carbon Capture Simulation Initiative, where he presented a poster paper on “Superstructure Optimization for Carbon Capture Process” and demonstrated related GAMS/BARON software. Also in October, he attended the annual INFORMS meeting, where he chaired a session on “Surrogate and Derivative-free Optimization.” He and his students presented five papers at INFORMS, on various topics in the areas of global optimization, derivative-free optimization, and carbon capture. Nick also served as reviewer on an NSF panel for CAREER awards. In December, Nick visited IBM TJ Watson research lab, where he gave a talk on “Third Generation Branch-and-reduce Codes Algorithms for Global Optimization of Nonconvex NLPs and MINLPs.” Also in December, Nick was selected as a member of the first Governing Council of the University of Macedonia, in Thessaloniki, Greece.

Erik Ydstie is one of the 5 Trustees of the FIPSE (Future Innovations in Process Systems Engineering). The first conference of the FIPSE took place near Olympia, Greece, in August, 2012. There were about 50 participants who discussed process systems advances in nano-technology, pharmaceuticals and state estimation. In September Erik gave a 5 day short course on Adaptive Control at ETH in Zurich. He presented the same class at NTNU in Norway in October. Erik has started the organization of the 1st IFAC Workshop on Thermodynamics and Mathematical Systems Theory to take place in Lyon July 14-16, 2013. He has started writing a book on adaptive control to be co-authored with Dr. Laurant Praly at Ecole National Supérieure des Mines de Paris. The paper, “Solar Silicon Production,” authored by Ranjan, Balaji, Panella and Ydstie (published in *Computers and Chemical Engineering*, Vol. 35, p 1439-1453) won the 2011 best paper award.

Staff News

Laura Shaheen received the CIT 20 Years Length of Service award at the CIT Staff Recognition Ceremony on January 8, 2013. **Dean Jim Garrett** present the award to **Laura Shaheen**.



Visiting Scholars

Mr. Hubert Hadera from ABB AG in Germany is working with Prof. Ignacio Grossmann's group on the development of mixed-integer programming models for the optimal demand-side management of power-intensive processes.

Dr. Yijun He from Shanghai Jiao Tong University, China, is working with Prof. Nick Sahinidis's group on the development of optimization models and algorithms for electrochemical process systems..

Dr. Johannes Jaeschke from Norwegian University of Science and Technology, Norway, is working with Prof. Larry Biegler's group on dynamic optimization for chemical process operations.

Dr. Aipeng Jiang from Hangzhou Dianzi University, China, is working with Prof. Larry Biegler's group on process optimization, including topics such as multiscale modeling and optimization of large scale process systems.

Mr. Matthieu Riva, from Universit'e de Bordeaux, France, is working with Prof. Neil Donahue's group on the production of organic aerosol haze from the photo oxidation on polyaromatic hydrocarbons.

Ms. Edna Soraya Lopez Saucedo from Universidad de Guanajuato in Mexico is working with Prof. Ignacio Grossmann's group on modeling and simulation of reactive dividing wall distillation column.

Mr. Michael Tippett from The University of South Wales, Australia, is working with Prof. Erik Ydstie's group on dissipative distributed MPC.

Undergraduate News

COMMENCEMENT 2013!

Carnegie Mellon's 116th commencement will take place at 11am on Sunday, May 19th in Gesling Stadium (rain or shine). The procession of candidates across campus will begin at 10:15am. Guests are asked to be seated in the stadium by 10a.m. The ceremony will begin at 11am and last about 75 minutes.

The Chemical Engineering department ceremony will begin immediately following the university ceremony at The Carnegie Lecture Hall in The Carnegie Museum. After the ceremony, a special reception will be held at Phipps Conservatory for graduates and their guests.

The Doctor's hooding ceremony will take place at 8 p.m. on Saturday, May 18th in the Wiegand Gymnasium in the University Center. Doctor's candidates, participating faculty and other ceremony participants will robe in Rangos Hall (second floor, University Center) at 7:00pm and begin to process at 7:45pm. Doctor's candidates and faculty members should have confirmed their participation.

Be sure to follow the schedule of events and latest news at the commencement web site <http://www.cmu.edu/commencement/>.

If you have any questions about the university commencement ceremony, send an e-mail to commencement@andrew.cmu.edu. If you have questions about the departmental ceremony, contact Cindy at cp32@andrew.cmu.edu or stop by to see her in DH 1101.

Farewell

Farewell to the exchange students who spent the 2012-13 school year with us!

From RWTH Aachen in Germany: **Tian Lan, Mogan Ramesh, and Christoph Westerwalbesloh.**

From Imperial College in London: **Jason Cheng, Xian Bin Chua, and David Garnsey.**

We have enjoyed meeting all of them and bid a fond farewell!

Good Luck!

Our Yonsei University exchange students (**Soo Ah Jin and Jiwon Lee**) will rejoin us in the fall semester.

We also send our best wishes with the following students who will be studying abroad in the departmental exchange program for the 2013-14 academic year:

To Imperial College in London: **Caitlin Streamer, Malavika Thottappillil, Krithiknath Tirupapuliur, Samuel Winslow, Ariana Zito-Wolf**

To RWTH Aachen in Germany: **Christine Westcott**

To Technische Universität Dortmund in Germany for the Summer 2013 semester: **John Taormina**

Class of 2016

Welcome to the following first-year students who have chosen to join the Chemical Engineering Department.

Iyinoluwa Akinlabi-Oladimeji
Corrine Bacigal
Joetsaroop Bagga
Jonathan Berman
Michael Booker
Luke Bruce
Brooke Carter
Maggie Chen
Seyonna Christian
Benjamin DuCarme
Isaiah Edmonds
Edna Fongod
Will French
Daniel Galicia
Teresa Gelles
Christopher Hapchuk
Yoyinsola Ibikunle
Sophie Jung
Do Hyung Kim
Eleanor Kwik
Peter Lemaire
Danielle Maly
Brigid McGovern
Trevor Meeks
Alexandra Mod
Marissa Morales

Ishan Nag
Alexandra Newby
Sanjana Padmanabhan
Priya Patel
Santosh Prabha
Carrie Qiu
Kira Ragazzo
Dhrisya Raman
Vasilios Sahinidis
Christopher Schuler
Wooram Seok
Michael Shimko
Adam Simpson
Kira Singhaus
Daniel Sogunro
Elizabeth Starck
Holly Stokes
Zhuopin Sun
Zofia Tillman
Vishal Vala
Sirena Wang
Leah Willis
Sihui Wu
Jason Yan
Christia Zheng



Congratulations to the following students who are expected to be awarded their degrees on May 19, 2013:

Seniors

Kathleen Bates

Additional Major: Biomedical Engineering

Minor: German Studies

Hau Chen

Melanie Chin

Minor: Economics

James Church

Additional B.S.: Computer Science

Kelli Coffey

Additional Major: Biomedical Engineering

Anthony Difrancesco

Erin Donnelly

Stephanie Engel

Minor: Colloids, Polymers and Surfaces

Francisco Escobar

Minor: Colloids, Polymers and Surfaces

Gregory Fillios

Additional Major: Biomedical Engineering

Rocio Garay

Minor: Colloids, Polymers and Surfaces

Joshua Glagola

Minor: Music Technology

Benjamin Hauser

Minor: Colloids, Polymers and Surfaces

Russell Hensley

Additional Major: Engineering and Public Policy

Tiffany Ho

Additional Major: Biomedical Engineering
Minor: Music Performance

Kelsey Holstein

Jyo Lyn Hor

Minor: Materials Science and Engineering

Emerson Hum

Additional Major: Biomedical Engineering

Kevin Iacovino

Carissa Iannone

Additional Major: Biomedical Engineering

Ina Joo

Additional Major: Biomedical Engineering

Yong Ha Jung

Additional Major: Biomedical Engineering

Seung Hwan Jwa

Jessica Kafka

Nicholas Karabin

Additional Major: Biomedical Engineering

Richa Khosla

Carol Kim

Additional Major: Engineering and Public Policy
Minor: Global Systems Management

Sujung Kim

Additional Major: Biomedical Engineering

Price Kinney

Minor: Business Administration

Nancy Ko

John Lawlor

Additional Major: Biomedical Engineering

Katherine Lee

Double Major: Biomedical Engineering

Seung Lee

Stacey Lee

Double Major: Biomedical Engineering

Peggy Lees

Double Major: Biomedical Engineering

Minor: Music Theory

Adam Leibowitz

Minor: Colloids, Polymers and Surfaces

Charles Leung

Double Major: Technical Writing

Jack Li

Additional Major: Biomedical Engineering

Albert Liang

Minor: Environmental Engineering and Sustainability

Hector Lo

Additional Major: Biomedical Engineering

Chidi Mbaruguru

Sarah McCormick

Minor: Linguistics

Duke Miller

Additional Major: Biomedical Engineering

Zeinab Mohamed

Additional Major: Biomedical Engineering

Hiroataka Nakagawa

Double Major: Biomedical Engineering

Neha Nandakumar

Double Major: Engineering and Public Policy

Priyanka Nawathe

Minor: Materials Science and Engineering

Minor: Psychology

Tufale Nawaz

Minor: Business Administration

Minor: Environmental Engineering and Sustainability

Annelie Niebuhr

Minor: Chinese Studies

Nathaniel Ondeck

Additional Major: Biomedical Engineering

Soo Hyun Park

Additional Major: Biomedical Engineering

Lisa Rising

Double Major: Biomedical Engineering

Harrison Rose

Double Major: Biomedical Engineering

Aisulu Sagitova

Abigail Schaeffer

Joseph Selinger

Mala Shah

Additional Major: Biomedical Engineering

Yi Shi

Additional Major: Biomedical Engineering

Mark Wong Siang Kai

Additional B.S.: Computer Science

Edward Smongeski

Minor: Colloids, Polymers and Surfaces

Minor: Computer Science

Allen Song

Additional Major: Economics

Minor: Business Administration

Neil Soni

Double Major: Biomedical Engineering

Breanna Stillo

Double Major: Biomedical Engineering

Stephanie Stras

Double Major: Biomedical Engineering

Edmund Tang

Minor: Colloids, Polymers and Surfaces

Marianne Thaila

Additional Major: Biomedical Engineering

Sharanya Venkat

Additional Major: Biomedical Engineering

Minor: Business Administration

James Weltz

Additional Major: Biomedical Engineering

Chan-Mi Yang

Additional Major: Biomedical Engineering

Minghui Zhang

Additional Major: Biomedical Engineering

Minor: Physics

Minor: French and Francophone Studies

PhD Students

Cheng, Vicki

Title: Structure, Mechanics, and Transport in Block Copolymer-nanoparticle Composites at the Macroscopic and Nanometer Lengthscales

Advisor: Prof. Walker

Demeter, Ethan

Title: The Promotion of Base Metal Catalysts for the Electrochemical Oxygen Evolution Reaction

Advisor: Prof. Kitchin

Gupta, Vijay

Title: Modeling and Computational Strategies for Optimal Oilfield Development Planning under Fiscal Rules and Endogenous Uncertainties

Advisor: Prof. Grossmann

Jones, Angela (Holmen)

Title: Rapid Separations of Kilobase-Sized DNA using Micelle Size-Sampling

Advisor: Prof. Schneider

Lee, Anita

Title: A Multi-Scale Approach to Developing Solvents for Carbon Capture

Advisor: Prof. Kitchin

Meade, Jonathan

Title: High Yield Deregulated Plasmid DNA Production in *Escherichia coli* Characterized by Proteomics and Metabolic Flux Analysis

Advisor: Prof. Domach

Mhatre, Bharat

Title: Super-enantiospecific Autocatalytic Decomposition of Tartaric Acid and Aspartic Acid on Cu Surfaces

Advisor: Prof. Gellman

Panella, Rocco

Title: Construction and Modeling of Dye-Sensitized Solar Cell Photoanodes

Advisor: Profs. Prieve & Ydstie

Reichart, Matthew

Title: Using Microscale Interfaces to Connect Transport Dynamics, Interfacial Mechanics, and Coalescence Behavior for a Model Oil-Dispersant-Aqueous System

Advisor: Prof. Walker

Rock, Reza

Title: An Imaging Ammeter for High Throughput Electrochemical Research

Advisor: Profs. Prieve, Sides

Smith, Robert

Title: Multiscale Modeling Methodology: From Atomistic to Molecular and Beyond

Advisor: Profs. Biegler, Jhon

Wirth, Stacy (Pustulka)

Title: Impacts of Silver Nanoparticles on Bacterial Biofilms

Advisor: Prof. Tilton

Zorn, Keith

Title: Exploitation of Intermediate Structures for Simultaneous Convexification in Global Optimization

Advisor: Prof. Sahinidis

MS Students

Alothman, Ahmad

Title: Bi-criterion Optimization Planning Model for Process Networks with Multiple Scenarios and Environmental Impact

Advisor: Prof. Grossmann

Ding, Zhizhong

Title: Metal Oxide Oxygen Carriers for Chemical-Looping Combustion

Advisor: Profs. Kitchin/Miller

MChE Students

Chen, Hau

Dixon-Ernst, Alexandra

Hor, Jyo Lyn

Shah, Amit

Shah, Chaitanya

MS CPS Students

Jones, Angela (Holmen)

Shah, Pratik

Faculty Profile: Susana Chin Steppan

Hello! My name is Susana Chin Steppan. Even though I'm a recent addition to the department's faculty, I have been part of the CPS staff since 2004, when Annette Jacobson asked me to join her group. As of last September, I was appointed a full-time Assistant Teaching Professor and the official academic advisor to the Masters students.

Prior to coming to CMU, I held several industrial positions around the Pittsburgh area. My husband Dave and I moved to Pittsburgh's North Hills 23 years ago, and my first position was at Bayer Corporation, which in those days was called Mobay.

I was hired to manage part of the large characterization group within Polyurethane Research. My group, which consisted of 3 lab technicians and me, was in charge of the rheological characterization and thermal analysis of many of the products and materials produced not only in Polyurethanes, but also in the Plastics, Coatings and Adhesives, and Pigments and Optical Brighteners divisions. I was part of a number of teams working on projects that ranged from modifying the PU resins used for bowling balls to dampen bounce, developing elastomers for skateboard wheels, studying the flow during cure of powder coatings for automotive interiors, and improving the "feel" of cell phone cases for Motorola, to name a few. My budding career at Bayer was cut short by the birth of our daughter Carla in 1994. I



enjoyed stay-home mom status for a little while, until I heard PPG was looking for a rheologist!

I was hired by PPG Industries, Coatings and Resins Division, in 1996 and worked at their Research Center located in Allison Park. Even though I started out as their in-house rheologist, I promptly moved to the formulation side of the business, which I found fascinating. Coatings are extremely complex colloidal systems and balancing their ultimate properties is a tremendous challenge. After I learned to formulate, spray, and test automotive coatings, I was promoted to project leader of the Medium Solids Solventborne Automotive Clearcoats business. The medium solids automotive coatings market supplies most of Europe, Asia and Latin America.

During my tenure in this position, we commercialized the clearcoat that is currently used on the new VW Beetle. Next time you see one, check out its beautiful shiny topcoat! I was also co-inventor of a rheology modifier that served not only to control paint flow, but improved metallic flake orientation which is the key contributor to basecoat appearance. Although I loved the work at PPG, I found myself resigning my position when I was asked to move to Europe for 6 months to oversee the start-up of a paint line for PSA Peugeot Citroën. My daughter was still in elementary school and my husband might have noticed my 6 month absence!

While volunteering at my daughter's school and doing PTO work was very rewarding, I found my brain was atrophying from disuse. So one day I had the brilliant idea of re-inventing myself and joining the field of Art Conservation. The amazing thing is that I convinced the director of the Art Conservation Center at the former Mellon Institute to let me join them as a Visiting Scholar. I was there for almost 3 years when Annette Jacobson convinced me that my time was better spent contributing to the CPS program.

On a personal note, I was born and raised in Mexico; in the historic city of Oaxaca. I left home 31 years ago to come to the States for my college education. I lived in Los Angeles while obtaining my B.S. degree at the University of Southern California. While at USC, I did independent research with Dr. Theo Tsotsis on surface diffusion in porous catalysts, and decided I really liked doing experiments and working in the lab. So after graduating, I applied for graduate school and was accepted at the University of Massachusetts at Amherst. As much as I had enjoyed my catalysis work, my interest had shifted to polymers and I was thrilled to be at UMASS where they have one of the best Polymer Science and Engineering departments! I chose Dave Hoagland as my thesis advisor because he offered me a project that was the perfect balance between classical fluid dynamics and the fundamental physical chemistry of macromolecules. To this day I'm still an experimentalist at heart and I'm in my element when working in the lab surrounded by instruments and equipment. If you want to discuss experiments and/or characterization techniques, you can find me in DH#3101 or, better yet, the CPS labs.