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T I N Y  P A R T I C L E S
Big Impact

Carnegie Mellon University
Dear Alumni and Friends,

As the summer draws to a close, it is a pleasure to share some news of the Chemical Engineering Department over the past academic year. I am glad to report that the department is in excellent shape with strong directions for improvement on both research and educational fronts.

With almost 300 undergraduates and 200 graduate students, the Chemical Engineering Department is the third largest in the College of Engineering. We currently have 20 faculty members and 14 staff. On the research front we represent five areas: Bioengineering, Complex Fluids Engineering, Catalysis and Surface Sciences, Environchemical Engineering and Process Systems Engineering. This issue reports on the educational and research activities, achievements and recognitions of our faculty. I am especially glad to have such strong and dynamic faculty as colleagues.

This issue also contains three feature articles that describe exciting new developments in our department. Profs. Annette Jacobson and Rose Frollini describe our department’s very active K-12 outreach program with Pennsylvania schools as well as the Carnegie Science Center. Their work has strongly promoted interest in STEM fields, particularly in chemistry and chemical engineering. Prof. Katie Whitehead describes her work on therapeutic drug delivery. Her interdisciplinary research combines small molecule and polymer chemistry, nanoparticle characterization and materials interactions in living systems. A key focus of this work is to develop more patient-friendly means of administering injectable drugs, such as insulin. Her feature article describes the research challenges associated with development of an alternative oral delivery system. The article by Prof. Aditya Khair describes the development and application of mathematical techniques, from asymptotic analysis and numerical computations, to investigate problems in fluid dynamics, colloid science, rheology, electrochemistry and electrokinetics. His fundamental work has important impacts on breakthrough technologies that have come into our daily lives, from organic semiconductors (such as OLEDs) to fluid mechanics of swimming organisms, relevant to bio-mixing and bio-inspired propulsion. Moreover, a fundamental understanding of the dynamics of physical transport phenomena, coupled with experimental validation and refinement by our CFE colleagues, continues to enable novel technologies and applications.

Moreover, I am especially proud of our graduating undergraduate and graduate classes and their numerous achievements described in this issue. Among these awards, two of our undergraduates and John Berg scholars, Himali Rinade and Alexandra Cerny, won 1st and 2nd place awards, respectively, in the National AIChE undergraduate student poster competition. In addition, the CMU ChemE Car Competition team distinguished itself at the AIChE Mid-Atlantic Regional Conference last April. They will compete in the national competition at the AIChE Annual Student Conference. We look forward to celebrating with our students, colleagues — and you — in November. So please join us for the upcoming AIChE Annual Meeting, to be held in San Francisco from November 13-18.

Finally, special thanks go to our departmental staff and faculty colleagues, who continue the high level of performance in the department. I especially appreciate their experience in covering all of the bases over the past year. Along with the dynamic research and educational activities of our faculty, researchers, visitors and students, it is a great privilege for me to recognize all of the hard work of our faculty and staff.

Larry
Many years ago, when I was a second semester sophomore at the University of Delaware, I tentatively stepped into the office of my academic advisor and told him I no longer wanted to be a chemical engineer. My advisor, Dr. Jon Olson, smiled at me kindly, as always, and asked why someone so good at chemical engineering would want to switch majors. I explained that I couldn’t imagine a career in which I fitted pipes or spent my days hunched over a desk, deep in the throes of virial coefficient calculations.

Dr. Olson knew then what I didn’t — that chemical engineering is much more than the contents of our fluid mechanics and unit operations textbooks. Chemical engineering is a mindset, it’s a way of thinking. Instead of pigeonholing us, its sophistication and power are readily applied to many disciplines, ranging from oil manufacturing to consumer products to biotechnology. Dr. Olson diverted my attention from my unsavory coursework by involving me in protein research, and promised me that I could do whatever I wanted when I went to grad school.
Nanoparticles (green) for oral drug delivery need to cross the intestinal barrier before being absorbed into the bloodstream for delivery throughout the body.

So here I am, years later, behind my desk in Doherty Hall, with two Chemical Engineering diplomas on my wall. My amazement for the human body has led me to a career focused on drug delivery, which is the science of packaging up therapeutic drug molecules for safe and effective treatment. My lab is the definition of interdisciplinary: we do small molecule and polymer chemistry, characterize nanoparticles and study our materials in living systems. Chemical engineering is a way of thought in our research — it gives us the confidence to draw upon knowledge from disparate disciplines and the insight to view our delivery vehicles (a “unit”) in the context of the entire body (a “chemical plant”).

Drug delivery comprises two major goals: one is to take injectable drugs that are currently FDA-approved and to develop more patient-friendly means of administering them. Of my ~8 graduate students, half of them engineer oral delivery systems for macromolecular drugs. As an example, insulin is a protein drug that Type I diabetics must self-inject several times a day. To circumvent this painful therapy, our goal is to deliver proteins like insulin orally. Because our gastrointestinal tract’s job is to break down proteins, whether in food or therapeutics, we need to develop clever ways of protecting the protein drug from degradation in the stomach. Once the drug then reaches the intestine, it must overcome the most daunting hurdle: absorption across the intestinal wall into the bloodstream. To accomplish this, one of our strategies is to grow polymer chains off of the surface of the protein drug. We design these polymer chains with specific chemistry that sterically hinders enzymatic degradation of the protein while facilitating intestinal permeability and protein delivery into the bloodstream.

The second major goal of drug delivery is to design delivery vehicles for drugs that are not yet FDA approved (e.g., recombinant proteins, DNA and RNA medicines). We focus specifically on two forms of RNA delivery. Messenger RNA (mRNA) is a drug that encodes proteins, which we can use to treat diseases triggered by missing proteins. An example of this is hemophilia, which is caused by

Lipidoids (structure in a) are combined with several other ingredients, including the drug (siRNA) to form b) lipidoid nanoparticles. c) A cryo-TEM micrograph shows nanoparticle structure and size. d) Lipidoid nanoparticles (yellow) deliver siRNA into cancer cells.
the absence of a blood clotting protein normally produced by the liver. We are also experts on short interfering RNA (siRNA), a drug that turns off the production of proteins that are overexpressed in certain diseases (e.g., high cholesterol, Hepatitis B). Although these gene-based medicines are some of the most broadly powerful therapeutics ever discovered, their application is limited by an inability to deliver them selectively to diseased cell and organ targets. As we design our delivery vehicles in the form of nanoparticles, we ask — is there a way to deliver RNA only to a tumor while avoiding uptake into the liver, spleen and kidneys?

We believe one answer lies in our lipid nanoparticles. These are highly modular liposomal vesicles that include an aqueous core, which is the perfect depot for hydrophilic drugs such as RNA. The lipid bilayer exterior of our nanoparticles facilitates fusion with chemically similar cell membranes, and the amine content of the bilayer dictates drug release into the “heart” (cytoplasm) of the target cell. The nanoparticle surface can be further modified with targeting ligands that improve uptake into select cells within the body. These lipid delivery vehicles, which I originally designed as a postdoc, have thus far resulted in three patents that have been licensed by four pharmaceutical and biotech companies and have inspired the creation of an additional two companies. While my previous research focused on RNA delivery to the liver, my lab is currently expanding the application of lipid nanoparticles for the treatment of lymphoma, inflammatory bowel disease and diabetic wounds.

Cancer is formidable, and its effective treatment requires a multifaceted approach that attacks cancer cells using several mechanisms. Because many types of cancer are fueled by growth-encouraging proteins called oncoproteins, siRNA drugs can be used to reduce or turn off their expression. Work in our lab specifically centers on the treatment of Mantle cell lymphoma, a deadly type of Non-Hodgkin B cell lymphoma that kills most patients within five years of diagnosis. This is a disease in dire need of new therapies. We are using a cocktail of our nanoparticles to silence a trio of problematic genes characteristic of Mantle cell lymphoma. We’ve been delighted to find that our therapy kills 80% of cancer cells and significantly suppresses tumor growth in a mouse model of lymphoma. Our current efforts seek to divert more of the nanoparticles away from healthy tissue to reduce side effects while maximizing efficacy in the tumor. Ultimately, we anticipate that our siRNA-based nanoparticle therapies will be used to treat lymphoma in conjunction with the FDA-approved chemotherapies and immunotherapies already in place. It is our hope that our contributions to science, as chemical engineers, will improve and elongate the lives of patients in need of better therapies.
I joined the Chemical Engineering department in August 2010 as an assistant professor. Actually, rather than “joined” I should say “rejoined,” since I was at CMU in 1999-2000 as an exchange student from Imperial College London. Interestingly, I took a number of classes taught by my current colleagues! I have been an associate professor since 2015. My research group utilizes applied mathematical techniques, including asymptotic analysis and numerical computations, to investigate problems in fluid dynamics, colloid science, rheology, electrochemistry and electrokinetics (figure to right). We work on an array of topics, from charge transport in organic semiconductors (relevant to OLEDs) to the fluid mechanics of swimming organisms (relevant to bio-mixing and bio-inspired propulsion). That said, the unifying philosophy of our work is to rigorously quantify the dynamics of a physical transport phenomenon, with the aim of leveraging the gained knowledge to enable novel technologies and applications. A prominent feature is collaboration with experimentalists. We deliberately choose paradigmatic problems to elucidate the essential physics behind a flow or transport phenomenon. Described here are two central research themes in my group over the last few years.

Phoretic Motion of Colloids: Colloidal particles (which are typically a micron in size and thus affected by Brownian motion) can be transported through liquids by electric fields. Such electrophoretic transport is the workhorse of analytical chemistry and bio-separations, and is attractive in microfluidics. The central question: how fast does a particle move under an electric field? Put differently, what is the electrophoretic mobility, i.e., the velocity per unit field? The ability to accurately predict the mobility is paramount to microfluidic technologies and separation schemes. My work in this area has made advances for electrophoresis in concentrated, charge-laden media under large voltages.

Notably, the vast majority of existing work on electrophoresis has assumed that the electrical double layer (EDL) that forms spontaneously around a charged particle is described by the Poisson-Nernst-Planck (PNP) paradigm of point-sized, non-interacting ions. This cannot describe the EDL structure in concentrated electrolytes, ionic liquids and molten salts. Moreover, the PNP model leads to the predicted electrophoretic mobility being a non-monotonic function of the particle zeta potential (equivalent to particle charge), with a mobility maximum observed at intermediate zeta potentials. This has deleterious ramifications for the design of separations, as it suggests that two particles with different charges move at the same velocity. During my postdoctoral studies with Todd Squires at UCSB, I showed that the mobility maximum is an artifact of the impossibly large ion concentration predicted by the PNP model near a highly charged surface. Further work quantified the enhancement of electrophoretic transport due to hydrodynamic slippage.

A new theory for electrophoretic particle motion in concentrated electrolytes (Stout and Khair, J. Fluid Mech. 2014). Squares are experimental data (Semenov et al., Phys. Rev. E, 2013), which measure electrophoretic mobility $\mu_e$ of a micron-sized polystyrene particle versus ionic strength for three electrolytes. In the trivalent electrolyte LaCl$_3$, the sign change in mobility indicates a reversal in the direction of particle motion: a positive value for $\mu_e$ at large concentrations implies that the negatively charged particle drifts toward a negative electrode. Our theory (open circle and line) has provided the first continuum-level framework to predict this phenomenon.
My interest in phoretic motion has continued at CMU. For example, electric fields are routinely used to transport particles in fluids whose flow behavior, or rheology, does not follow Newton’s ideal. There is, however, a lack of knowledge of electrokinetic flows in such complex (non-Newtonian) fluids. In collaboration with Lynn Walker, we have developed a model to compute the electrophoresis of particles in a complex fluid. We predict that electrophoresis in a complex fluid is particle size- and shape-dependent, in contrast to electrophoresis in a Newtonian fluid, which may provide a route to new protocols for particulate separations. More generally, phoretic motion is animated by an imposed gradient of a scalar field: e.g., solute gradients cause diffusiophoresis and thermal gradients drive thermophoresis. It is usually assumed that the scalar field evolves solely via diffusion. However, intuitively, as the colloid moves it sets up a fluid flow that advects the same scalar field that instigated its motion. We have quantified the effects of advection on the phoretic motion of colloidal particles, finding that advection leads to symmetry breaking in the motion of fore-aft asymmetric particles, and to pattern formation in suspensions, which is relevant to self-propelled colloidal motors.

We have recently developed a continuum theory for electrophoresis in concentrated multivalent electrolytes. This is motivated by experiments over several decades that show electrophoretic “mobility reversals,” where a positively charged particle migrates to a negative electrode at low ionic strength; after the ionic strength rises above a critical value the colloid migrates to the positive electrode — in apparent violation of Coulomb’s law! Our theory predicts a mobility reversal that compares favorably with experiments. Ours is the first purely continuum theory able to predict a mobility reversal: we identify that ion-ion electrostatic correlations are the root cause, an issue that has been debated extensively in the literature. Our work opens up a path to quantify a host of electro-kinetic and chemical phenomena in concentrated electrolytes and ionic liquids. In particular, we are developing an analogous continuum theory for diffusiophoresis in electrolyte gradients, motivated by oil recovery applications, where tailoring particle migration in concentrated brines is a potential route to “smart particles” that can sense oil-rich reservoir regions.

Rheology & Colloidal Hydrodynamics: I have been interested in rheology since my graduate studies. My graduate work developed theoretical paradigms for active microrheology of complex fluids. I demonstrated that the force on a driven colloidal “probe” particle could be interpreted as a “microviscosity,” which bears close resemblance to the shear viscosity determined from mechanical rheometry. As a postdoc, I proposed a new active microrheology technique to measure normal stress coefficients of complex fluids. This was the first instance in which active microrheology quantitatively recovers a nonlinear rheological property.

At CMU, our recent rheological work has quantified the motion of a colloidal probe driven through a sheared suspension. The ambient shear causes cross-streamline migration of the probe, which is the colloidal analog to inertial (Saffman) lift. Moreover, we predict drag reduction for a probe driven orthogonal to the shear flow. There has been recent interest in particle settling in orthogonal shear, which is relevant to hydraulic fracturing. Specifically, an orthogonal shear is used to delay the settling of “proppant” particles, allowing them to travel farther into a hydraulic fracture and thus keeping a larger portion of that fracture accessible. The mechanism for the alteration in drag under orthogonal shear is debated. Our work allows for a precise identification of the microscale processes that result in drag modification for colloidal fluids.

Finally, our group has recently gotten interested in large-amplitude oscillatory shear (LAOS) rheology of complex fluids. The aim of a LAOS experiment is to determine the nonlinear viscoelasticity of a material by exposing it to a strong, time-periodic deformation. We have developed a new theoretical framework to quantify LAOS dynamics at large strain amplitudes and large strain rates, which offers a unique perspective on nonlinear viscoelasticity. Our efforts are in contrast to existing work that is restricted to moderate strain amplitudes. For example, our approach offers new methods to infer nonlinear parameters in constitutive equations from oscillatory shear experiments. We are now developing a program to enable the results of a LAOS experiment to predict material rheology under other flows of arbitrary type (e.g., shear or extensional) and time-dependence (e.g., startup or cessation). This is particularly important for processing applications, wherein a material may be exposed to different flow types and intensities during various stages.
BRINGING plain text TO LIFE

by Hannah Diorio-Toth

John Kitchin, professor of chemical engineering at Carnegie Mellon University, has developed an open source software designed to improve data sharing in applications such as engineering education and scientific publishing. The software, called scimax, was created out of Kitchin’s own frustration with using clunky word processing and text editing software to write scientific papers.

“Right around the time I got tenure, I started looking at what the next 20 years of my research could look like if I stayed on the trajectory I had been on in my career,” says Kitchin. “I knew a lot was possible, but I felt like I’d hit a plateau in productivity. I couldn’t find any software out there that did what I needed, so I created scimax.”

The software uniquely integrates data processing and analysis directly into plain text. This integration brings plain text to life, allowing for a multitude of applications in research, teaching, and writing. For example, scimax streamlines the process of writing scientific papers and eliminates the need for using multiple programs like word processors, reference managers, and data/analysis plotting programs. The software does not require the user to know how to code, says Kitchin.

Kitchin recently published two papers about using scimax to increase data sharing and efficiency in scientific publishing. The papers include “Examples of effective data sharing in scientific publishing,” published on May 11, 2015 in ACS Catalysis, and “Automating data sharing through authoring tools,” published on June 11, 2016 in the International Journal on Digital Libraries.

For more information on scimax, please visit John Kitchin’s website at kitchingroup.cheme.cmu.edu/scimax.
Larry Biegler, along with Ignacio Grossmann and Nick Sahinidis, gave a plenary talk in May 2016 at the American Russian Chemical Engineering Summer School held at the Kazan National Research Technological University in Kazan, Russia. This school is held to foster further collaboration, development and experience exchange between Russian and American scientists. The research discussions covered development and application of the methods/approaches in computer modeling and optimization of chemical processes. Also, at the Annual 2015 AIChE meeting, he received the William H. Walker Award for Excellence in Contributions to Chemical Engineering Literature.

Neil Donahue has been recognized in the field of Geosciences by Reuters in a publication called “The World’s Most Influential Scientific Minds” as a highly cited researcher based on his respective output of top-cited papers in his field. This publication features researchers who have won acclaim and approval among their peers.

Kris Dahl, along with collaborator Prof. Mohammad Islam of CMU’s Department of Materials Science & Engineering, presented her work on using carbon nanotubes for drug delivery at the Carbon Nanostructures in Medicine and Biology Symposium of the Electrochemical Society conference in 2016. Kris has also been cited as one of the scientists in engineering’s World Cancer Day presentation due to her work in how to stiffen the nucleus of cancer cells to stop their metastatic potential. In addition, she was a guest editor for a Special Topic on Nuclear Mechanobiology for “Cellular and Molecular Bioengineering,” a journal of the Biomedical Engineering Society.

Andy Gellman has received a three-year grant from the National Science Foundation to support a study on “Acetylene Hydrogenation on Alloy Catalysts Spanning Ternary Alloy Composition Space.” Finding the alloy composition that optimizes the removal of acetylene from ethylene is critical to improving the efficiency processes that ultimately convert ethylene to higher value chemicals.

He also spoke at the Weizmann Institute of Science in Israel at a symposium entitled “80 Years of Self-assembly and Chirality.”

Chrysanthos Gounaris co-authored a paper “Multi-stage Adjustable Robust Optimization for Process Scheduling under Uncertainty,” which was the May 2016 selection for the Editor’s Choice Paper of the AIChE Journal.

Ignacio Grossmann was awarded an Honorary Doctorate from the Kazan National Research Technological University in Kazan, Russia. He also was an organizer of the American Russian Chemical Engineering Summer School, which fosters further collaboration, development and experience exchange between Russian and American scientists.

He was granted another Honorary Doctorate from the University of Cantabria in Santander, Spain, for the excellence of his research work and his international impact in the field of chemical engineering.

Ignacio also gave a two-day short course at King Abdullah University of Science and Technology in Thurwal, Saudi Arabia, on “Mixed-integer and Disjunctive Programming and Mixed-integer Models for Planning and Scheduling.”

In addition, he delivered the Distinguished D.B. Robinson lecture, “The Increasing Scope of Optimization in the Oil and Gas Industry,” at the Department of Chemical and Materials Engineering of the University of Alberta in Edmonton, Canada.

Ignacio has been recognized in the field of Computer Science by Reuters in a publication called “The World’s Most Influential Scientific Minds” as a highly cited researcher based on his respective output of top-cited papers in his field.

Aditya Khair has been selected as the 2016 Camille Dreyfus Teacher-Scholar in recognition of his outstanding work in suspension rheology, physico-chemical hydrodynamics, micro-rheology and electrokinetics. Recipients of the Camille Dreyfus Teacher-Scholar Awards are selected primarily based on individual research attainment and promise, along with evidence of excellence in teaching.

Aditya also gave a talk entitled “Changes, Forces and Particles in Ionic Liquids” at the Kaufmann Foundation symposium held in Pittsburgh.
Spyros Pandis has won the Lawrence K. Cecil Award in Environmental Chemical Engineering from AIChE. His research applies principles of chemical engineering to the control of air pollution and climate change. His 230 peer-reviewed papers have received approximately 14,000 citations. The work of his group has contributed to successful regulation and improvements in air quality in various areas around the world.

Nick Sahinidis, along with Larry Biegler and Ignacio Grossmann, gave a plenary talk in May 2016 at the American Russian Chemical Engineering Summer School held at the Kazan National Research Technological University in Kazan, Russia. This school is held to foster further collaboration, development and experience exchange between Russian and American scientists. The research discussions covered development and application of the methods/approaches in computer modeling and optimization to solve issues in design, control and research of oil and gas refining, petrochemical processes and productions aimed at rational use of energy and raw material resources for the protection of the environment and sustainable development.

In addition to this, Nick gave a plenary talk at the 5th International Symposium and 27th National Conference of the Hellenic Operational Research Society (HELORS). At this conference Nick received the society’s 2016 National Award and Gold Medal.

Nick also gave a plenary talk at the European Symposium on Computer-Aided Process Engineering (ESCAPE) in Portorož, Slovenia.

Bob Tilton has received a three-year National Science Foundation grant for the project “Synergistic or Antagonistic Effects of Polymer/Surfactant Supramolecular Assembly on the Colloidal Depletion Force.” This research will determine how forces associated with the creation of self-assembled complexes of electrically charged polymers and surfactants can be manipulated to engineer performance characteristics of a wide variety of industrial complex fluids, including machining liquids, coatings and pharmaceutical dispersions.

Bob delivered the keynote address on the effects of polymer and surfactant complexation on surface tension driven “Marangoni” flows at complex fluid interfaces at the American Oil Chemists Society Annual Meeting in Salt Lake City. He collaborated in this work with Todd Przybycień (CHBE/BME), Steve Garoff (Physics) and post-doc Gunnar Duner. In addition, Bob presented seminars at both the Danish Technical University in Denmark and the University of Copenhagen Faculty of Health & Medical Sciences.

Lynn Walker has won the 2016 Barbara Lazarus Award for Graduate Student and Junior Faculty Mentoring. This award recognizes exemplary contributions to fostering a welcoming and nurturing environment for graduate students and young faculty at the university.

She was also the recipient of the 2015 AIChE Woman’s Initiative Committee Mentorship award.

In addition, Lynn has been elected as a Fellow of the American Institute of Chemical Engineers. Her research achievements cover a wide spectrum of fundamental and applied topics that contribute to the understanding of the structure and properties of soft material, spanning basic non-Newtonian rheology to surface properties.

Lynn presented an invited paper at the Nanoparticle Assembly Faraday Discussion organized by the Royal Society of Chemistry in Mumbai, India.

Lynn has also been named as the Editor-in-Chief of Rheologica Acta, one of the primary technical journals in the field of rheology.

Katie Whitehead was recognized on the cover story of Popular Science magazine as one the “Brilliant 10: honoring the brightest young minds reshaping science, engineering and the world.” Katie has been listed in the magazine as a scientist who “designs drugs to wipe out disease.”

She has also been selected as a 2016 Associate Scientific Advisor for “Science Translational Medicine.”

In addition, Katie was cited as one of the scientists in engineering’s World Cancer Day presentation due to her work with developing tiny particles called siRNA-loaded lipid nanoparticles that selectively enter and destroy lymphoma cells.

She has also been named a 2016 Young Innovator by the journal “Cellular and Molecular Bioengineering” (CMBE) which includes many of the best and brightest working in the field according to the CMBE editors. She will present her research at the 2016 Annual Biomedical Engineering Society Meeting in Minneapolis, Minn. October 5-8, 2016.
Outreach

Greg Martin (BS, ChemE 1976), Distinguished Engineering Associate at ExxonMobil, presents a check to Department Head Larry Biegler. The donation from ExxonMobil is to be used for educational purposes within the department of Chemical Engineering.

Colloids, Polymers and Surfaces (CPS) program director, Dr. Annette Jacobson and associate director, Rosemary Frollini have been involved in STEM outreach since the early 1990s, long before STEM was defined as an educational concept. Direction of students and teachers in inquiry-based activities was the basis of their efforts to spark the interest of K-12 students in science and engineering. Ten years ago, CPS assistant director, Dr. Susana Steppan, joined this effort.

Beginning first with in-school visits, and often inviting teachers and students to the PPG Industries CPS labs, they realized that their lab layout was not optimal for this type of instruction. With a grant from the PPG Industries Foundation in 1998, they remodeled one of their labs to more resemble a traditional classroom, while still keeping its functionality as a university teaching lab. Movable lab tables facing a blackboard and a drop-down projection screen provided this flexibility to welcome groups of varying sizes and ages.

Through the years, they and their student volunteers have participated in many university and community-related K-12 Outreach Programs on an annual basis such as Moving 4th (grade) Into Engineering, SWE High School Days, Engineering Your Future, SEE (Summer Engineering Experience), the Gelfand Center for Outreach Summer Sampler, Scouting for Engineers, and National Chemistry Week and National Engineers Week at the Carnegie Science Center. Jacobson and Frollini served as faculty members for the Group Pennsylvania Department of Education and MCS sponsored Governor’s Institute for Physical Science Educators (GIPSE), a professional development program for Pennsylvania state science educators with emphasis on inquiry-based science education.

Participating since its inception, their activities at the Carnegie Science Center have always been well received, often being included in publicity for the events. One memorable year, the theme for National Chemistry Week was “Behind the Scenes at the Movies.” Hundreds of student visitors were getting into the mood for
Halloween with ugly, oozing slashes on their arms, compliments of CPS volunteers and fake blood products of the type used by professional make-up artists, all the while learning about the composition and properties of gels.

Prof. Jacobson coordinated the first college-wide participation of the College of Engineering at Engineers’ Week at the Science Center. All engineering departments participate by sponsoring a table with hands-on activities related to each engineering discipline.

This program has continued annually since 2002, with volunteer participation ranging from 75-100 students, staff and faculty each year.

In the past 26 years, they have developed a diverse selection of exciting hands-on activities in polymer and forensic science that are available to all visitors at the Gelfand Center for Service Learning and Outreach website (www.cmu.edu/gelfand). Complete lesson plans, including pdf files, can be accessed by teachers for use in their classrooms.

Currently, Jacobson and Frollini have been instrumental in the creation of a engineering-wide STEM Committee and STEM website as the College of Engineering begins to coordinate the efforts of faculty who are involved in outreach activities to promote the broader impacts of their research programs. A new initiative for the STEM committee is the development of STEM kits that emphasize engineering principles that can be borrowed for classroom use by area teachers.

In the last few years, the Chemical Engineering Graduate Student Association (CHEGSA) organized a Graduate Student Outreach committee to provide a supply of interested volunteers to assist with the activities. These students gain experience in teaching, presenting to diverse audiences and learning how to express science and engineering concepts to the public. As they graduate and begin their careers, they take their experiences with CPS Outreach with them for their own programs, further extending the reach and impact of our program.

Prof. Jacobson summarizes the motivation for their work, “The Colloids, Polymers and Surfaces (CPS) educational program is currently celebrating its 43rd year at Carnegie Mellon University. Our outreach program is an essential part of this educational program that promotes science and engineering concepts and careers to K-12 students, educators and the public while also providing valuable volunteer opportunities for our students, faculty and staff. These collective efforts make it possible to accomplish our mission of providing science and engineering education to a wide audience.”
AIChE Annual Meeting will be held this year in **San Francisco** on November 13-18, 2016.

Above are some of our alumni enjoying the Chemical Engineering reception at last year’s meeting in Salt Lake City.
CAPD Annual Review Meeting

The latest successful Annual Meeting of the Center for Advanced Process Decision-making took place on March 7-8, 2016. It was preceded by the meeting of the Energy Systems Initiative group on March 6, and followed by the meeting of the group on Enterprise-wide Optimization on March 9-10. The group had a total of 39 participants from the process industry. Copies of the slides of the meeting are available at capd.cheme.cmu.edu/newsletters.html.

The CAPD Short Course (Conceptual Design, Optimization Modeling and Integrated Process Operations) was held May 4-11, 2016. The short course is organized into three parts consisting of seven modules, which can be taken in any combination (e.g., one, two, three or all seven):

I. Conceptual Design focuses on creation of superior process concept alternatives:
   • Process Synthesis (Sirola)

II. Optimization Modeling focuses on modeling and algorithms with applications to process optimization, process synthesis and molecular design:
   • Nonlinear programming (Biegler)
   • Mixed integer and disjunctive programming (Grossmann)
   • Global optimization and optimization under uncertainty (Sahinidis)

III. Integrated Process Operations focuses on three major decision levels in plant and enterprise-wide optimization:
   • Mixed-integer models for planning and scheduling (Grossmann)
   • Advanced Process Dynamics and Control (Ydstie)
   • Differential/algebraic models for real-time optimization (Biegler)

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 and the schedule for next year’s meeting may be found at capd.cheme.cmu.edu/shortcourse/index.html.

Enterprise-wide Optimization

egon.cheme.cmu.edu/ewocp/

The EWO meeting took place on March 9-10, 2016. The group currently comprises the following companies: ABB, Air Liquide, Air Products, Aurubis, Braskem, Dow Chemical, ExxonMobil, Petrobras, P&G, Praxair, SK Innovation and Total.

Pictured at left are Ignacio Grossmann (CMU), John Wassick (Dow), Iiro Harjunkoski (ABB), Pedro Castro (Univ. of Lisbon) and Carlos Mendez (INTEC, Argentina), the co-authors of “Scope for Industrial Applications of Production Scheduling Models and Solution Methods,” which won the 2014 Best Paper Award from the Computers and Chemical Engineering Journal. The award was presented to them at the AIChE meeting in November 2015, but all of the authors were present in our department for the Enterprise-Wide Optimization meeting held in October of that year. Other co-authors of the paper are Peter Bongers, Sebastian Engell, John Hooker, Christos Maravelias, and Guido Sand.
ChemE Car Competition Team Heading to Nationals in San Francisco!

The ChemE Car team competed at the Mid-Atlantic Regional Competition in April 2016 and their cars, Spare Parts and Chem-E-Car & Chill, won 2nd and 7th place. This November, the Spare Parts team will compete in national competition at the AIChE Annual Student Conference.

CHEM E OPEN HOUSES

Several Open Houses were held for potential ChemE Ph.D. candidates from around the world. A total of 42 students attended these three weekends.

Recent grad ALEXANDRA NEWBY (BS ChemE 2016) was one of three finalists for the George Washington Prize of the Engineers’ Society of Western Pennsylvania. This award strives to reinforce the importance of engineering and technology within our society and is given to a senior who demonstrates qualities of academic excellence, service and leadership. Alexandra is pictured with Dean James Garrett Jr.
Sixteen undergraduate students were fortunate to gain research experiences during Summer 2016 thanks to the generosity of several donors in conjunction with University, College, and Department funds. The summer undergraduate researchers also participated in the John Berg Undergraduate Research Symposium, which provided travel funds to the AIChE National Poster Competition.

Summer researchers and funding were as follows:

**Roy W. Weiland Undergraduate Internship in Chemical Engineering**
- Andres Ramirez – ChE/BME

**Roy W. Weiland Undergraduate Internship in Chemical Engineering and Undergraduate Research Office support**
- Rena Miu – ChE/BME

**Barry L. Tarmy Summer Research Internship Fund**
- Casey Salandra – ChE/BME

**Barry L. Tarmy Summer Research Internship Fund and Undergraduate Research Office support**
- Jacob Vries – ChE
- Jamie Vizelman – ChE/BME
- Adrian Berger – ChE/BME
- Christopher Lee – ChE/BME

**John C. Berg Undergraduate Research Scholars Endowed Fund and support from Chemical Engineering Faculty**
- Shrishti Kedia – ChE

**John C. Berg Undergraduate Research Scholars Endowed Fund and Undergraduate Research Office support**
- Jennifer Lott – ChE
- Shridhar Singh – ChE/BME

**Linda A. Halas E’75 Endowed Undergraduate Research Fund and Undergraduate Research Office support**
- Allison Kirkby – ChE
- Tamara Amin – ChE
- Felicity Gong – ChE/Math

**Jennings Summer Undergraduate Research Experience Awards**
- Dalia Laredo – ChE/BME
- Chukwudumebi Ogbogu – ChE

**Undergraduate Research Office**
- Matthew Carroll – ChE/Physics

An undergraduate research symposium poster session was held in September 2015 to select the Berg Scholars to represent our department in the AIChE Undergraduate Student Poster Competition. Junior Alexandra Cerny and sophomore Himali Ranade (pictured above) were chosen for the travel award, and honorable mentions went to senior Muyuan Li and sophomore Matt Palmer.

Congratulations to Himali Ranade, who won first place at the National AIChE competition for her project titled “siRNA Loaded Lipidoid Nanoparticles for the Treatment of Diabetic Foot Ulcers and Chronic Inflammatory States” and to Alexandra Cerny, who won second place for her project titled “Integration of Cellular Structures Modulate Motility and Response to Applied Force.”
Awards and Honors

AICHE PROFESSIONAL PROMISE AWARD
Recognizes an outstanding senior from each of the four regional programs in ChemE (CMU, University of Pittsburgh, West Virginia University and Youngstown State University), based on both their accomplishments as undergrads and their potential for achievement.

KEN WESTERBERG AWARD
Presented to the senior who has shown exceptional promise for research.

KEN MEYER AWARD
Presented to a doctoral student who has demonstrated excellence in graduate research in chemical engineering.

AMERICAN INSTITUTE OF CHEMISTS AWARD
The recipients of the American Institute of Chemists Foundation Award are selected on the basis of ability, character, scholastic achievement and professional potential.

KUN LI AWARD
This award is given to the Chemical Engineering faculty member who has the greatest impact on the graduating class and is selected on the basis of the senior class’s comments.

GEOFFREY PARFITT AWARD
The Geoffrey Parfitt Award is given to a graduating senior who demonstrates excellence in chemical engineering research.

McCABE AWARDS
These awards recognize undergraduate students who have distinguished themselves through exceptional service and noteworthy participation in activities that enhance the lives of the members of the department, the university and the community at large. This honor society celebrates the diversity of ways in which students may bring recognition to themselves and their communities, while pursuing the particularly challenging chemical engineering major.

MARK DENNIS KARL OUTSTANDING TEACHING ASSISTANT AWARD
Presented to a doctoral student who has demonstrated excellence as a teaching assistant in chemical engineering.

Left to right: student Maggie Chen and Prof. Susana Steppan.

Left to right: Joetsaroop Bagga, Jonathan Berman, William French, Eleanor Kwik, Alexandra Newby, Wooram Seok, Adam Simpson.

Left to right: Maggie Chen, Adam Simpson, Ben Yezer, Alex Newby.
The Distinguished Lecture Series Herb Toor Lectureship

Prof. Herbert Toor, whose 39-year career at CMU included roles as Chemical Engineering department head and dean of Carnegie Institute of Technology, was internationally known as a leader in diffusional mass transfer, multiphase processes and chemical reaction in turbulent flows. This lectureship, established in his honor, recognizes a distinguished member of the chemical industry who has been active in promoting closer links between industry and academia.

GAVIN TOWLER, who presented the Herb Toor Lectureship on March 31, 2016, is the vice president and chief technology officer at Honeywell Performance Materials and Technologies, a leading supplier of catalysts, process technology, proprietary equipment and services to the oil, gas and petrochemical industries. He co-authored Chemical Engineering Design, a textbook on process design, and is an adjunct professor at Northwestern University, where he teaches the senior design class.

Dr. Towler spoke on “Frontiers in Hydrocarbon Processing.” His presentation gave an overview of current trends in the hydrocarbon processing industries and their impact on technology development and selection. Recent innovations in oil and gas production technology have caused large swings in oil prices, leading to uncertainty in the markets, delayed investments and a dramatic reduction in employment opportunities in the oil and gas sector. The underlying trends that determine fuel consumption remain strong, and society continues to demand greater production of cleaner fuels. The oil and gas industry is responding by upgrading oil refineries and reallocating investment portfolios. Longer term, renewable fuels will continue to play an increasing role. Implications for researchers and technology developers were discussed.

U.S. Congressman KEITH ROTHFUS (PA 12th District), a relative of former Chemical Engineering faculty member Bob Rothfus, visited the department this March. Lab instructor MATT CLINE showed the Congressman the Robert R. Rothfus Undergraduate Laboratory, and the two shared a lengthy and pleasant conversation. The congressman particularly enjoyed Prof. Rothfus’ 1948 gradebook — a gradebook that clearly predates the grade inflation phenomenon! Alumna Kate Uncapher had a personal gift for Congressman Rothfus and he also left with a copy of Prof. Rothfus’ book, The History of Chemical Engineering at Carnegie Mellon, in which the warm, congenial nature of the man is evident. Congressman Rothfus was very pleased to see how his family legacy has been honored.
GEOFFREY D. PARFITT MEMORIAL AWARD FOR EXCELLENCE IN ORAL PRESENTATION | Qi Zhang

Geoffrey D. Parfitt, who was a professor of chemical engineering until his death in 1985, was internationally known for his contributions to the fields of colloid and surface science and powder technology. The ChEGSA students established this award, honoring the best student presentation at the ChEGSA Symposium, in his memory.

GARY POWERS POSTER AWARD | Khalid Hajj

Professor Gary Powers, a long-time faculty member of the Department of Chemical Engineering, was a well-known, leading researcher in process systems engineering, particularly in the area of process risk assessment and process synthesis. He developed theories and models for synthesis and evaluation of high integrity operating procedures, and novel approaches for the verification of real-time control systems, combining chemical engineering models with software engineering techniques.

His students, who frequently awarded him the “Kun Li Award for Excellence in Education,” appreciated Gary’s enthusiasm in the academic setting.

After Gary’s death in 2007, The Gary Powers Poster Award was established to continue his strong support of education.

This award is given to the student with the highest poster presentation score at the ChEGSA Symposium.

The 38th Annual ChEGSA Symposium will be held October 20-21, 2016.

The 38th Annual ChEGSA Symposium will be held on Thursday and Friday, October 20 and 21, 2016, so make sure to mark your calendar for this event!

MICHAEL F. DOHERTY, a member of the National Academy of Engineering and professor of Chemical Engineering at the University of California, Santa Barbara, will deliver the keynote address this year. Prof. Doherty’s background is in the area of process and systems engineering, but his current research interests have included: crystallization of organic materials, combining reactions and separations, and systems with complex chemistries. He was named one of the “One Hundred Chemical Engineers of the Modern Era (post 1945)” by AIChE in 2008.

In the meantime, keep an eye on the ChEGSA Symposium website (chegsa.cheme.cmu.edu/symposium/) for information. More details regarding the schedule, abstract deadlines and judging requests will be available as we get closer to the event.

In Memoriam

Dolores Dlugokecki passed away on March, 16, 2016, at age 85. Dolores is pictured with Prof. Andy Gellman at the celebration of her 40-year anniversary at CMU. She started here as a temporary secretary, intending to stay for a short period of time, but remained with us for a remarkable 44 years! Dolores will be remembered fondly by all for her small stature, feisty demeanor, great love for the Pittsburgh Steelers and her amazing loyalty to the Department of Chemical Engineering. She is survived by a daughter and three grandsons.
CLASS OF 2016


ROW 5: Prof. Michael Domach | Prof. Kris Dahl | Prof. Chrysanthos Gounaris | Prof. Neil Donahue | Prof. Todd Przybycien | Prof. Susana Steppan | Prof. Erik Ydstie | Prof. Robert Tilton | Prof. Aditya Khair | Prof. Annette Jacobson | Prof. Lorenz Biegler | Prof. Lynn Walker | Prof. Spyros Pandis | Prof. Ignacio Grossmann | Prof. Andrew Gellman | Prof. James Schneider | Prof. John Kitchin | Prof. Kathryn Whitehead
Recognitions for Our Loyal Alumni

Ester Marie Barbuto (ChemE 2008) of Booz Allen Hamilton, who is currently an MBA candidate at the University of Virginia, was named a Distinguished New Engineer by the Society of Women Engineers.

Michael Bevan (Ph.D., ChemE 1999), professor of chemical and biomolecular engineering at Johns Hopkins University, has been elected a 2016 American Chemical Society Fellow, recognizing his outstanding achievements in and contributions to science, the profession and ACS.

Jaime Cerda (ChemE 1980), professor of chemical engineering at the Universidad Nacional del Litoral and superior researcher at the Argentine National Scientific and Technical Research Council (CONICET), has been named recipient of the prestigious 2015 Recognition Award in Engineering from the National Academy of Science in Argentina in recognition of his contributions in the area of process systems engineering.

Lalit Chordia (ChemE 1985), president and CEO of Thar Energy, was elected to the American Association for the Advancement of Science in honor of his outstanding contributions leading to innovations of supercritical fluid technologies and for championing the widespread use of these technologies.

Jordan Green (B.S., ChemE/Biomed 2003), associate professor of biomedical engineering, ophthalmology, neurosurgery and materials science & engineering at Johns Hopkins University, will be presented with the Allan P. Colburn Award for Excellence in Publications by a young member of the American Institute of Chemical Engineers at the 2016 AIChE meeting. He has also been awarded the 2016 TERMIS (Tissue Engineering) Young Investigator Award from the TERMIS-AM conference.

Matt Helgeson (B.S., ChemE 2004) an assistant professor of chemical engineering at the University of California, Santa Barbara, has won the 2016 Unilever Award. This is given in recognition of fundamental work in colloid or surfactant science carried out in North America by researchers in the early stages of their careers. Previously, Helgeson has won awards from the National Science Foundation, the Department of Energy, the Northrup Grumman Excellence in Teaching and the Victor LaMer Award from ACS. His current area of research includes the engineering of colloidal particulates and gels, advanced separations and energy conversion.

Il Moon (ChemE 1992) was recently appointed as director of the National Science and Engineering Programs in NRF (National Research Foundation of Korea). In addition to that, he received an award from the president of South Korea, based on his LNG research and excellence in education.

Vipul Jain (Ph.D., ChemE, 1999) has been named head of the residential mortgage backed securities (RMBS) research team at Wells Fargo Securities, based in New York and Charlotte.

JitKang Lim (Ph.D., ChemE 2009) has received the Promising Academician Award of the Malaysian Ministry of Higher Education. Lim is an associate professor of chemical engineering at the Universiti Sains Malaysia. An expert in nanomaterials, Lim had been honored in 2014 with the National Young Scientist Award of the Malaysian Ministry of Science, Technology and Innovation, and is the first person in Malaysia to receive both honors. While at Carnegie Mellon, JitKang Lim’s Ph.D. research was co-advised by chemical engineering professor Bob Tilton and physics professor Sara Majetich.

Rebecca Liebert (Ph.D., ChemE 1995) has been named president and CEO of Honeywell UOP, a leading supplier of process technology, catalysts, engineered systems, and technical and engineering services to the global petroleum refining, petrochemical, chemical and gas processing industries.
Michelle O’Malley (ChemE, Biomed 2004), who is currently an assistant professor at the University of California, Santa Barbara, received the Presidential Early Career Award for Scientists and Engineers (PECASE). The award is the highest honor the nation can bestow on a scientist or engineer at the beginning of his or her career.

Jonathan Rothberg (ChemE 1985), Carnegie Mellon University trustee Jonathan Rothberg, whose groundbreaking work on DNA sequencing greatly increased the speed and efficiency of genome analysis, received the National Medal of Technology and Innovation. The medal is the nation’s highest honor for achievement and leadership in advancing the fields of science and technology. Rothberg is one of seven winners of the medal, which was awarded at a White House ceremony early this year.

Marvi Matos (ChemE 2006) of Boeing Research and Technology won the “Most Promising Engineer or Scientist (Advanced Degree)” award from the Hispanic Engineering National Achievement Awards Conference.

Paul McKenzie (Ph.D., ChemE 1992) has been appointed as executive vice president, Pharmaceutical Operations & Technology, of Biogen, Inc. In addition to leading the organization responsible for asset management, technical development, global manufacturing, supply chain operation, quality and engineering, he is overseeing construction and operation of Biogen’s advanced biologics manufacturing facility in Solothurn, Switzerland.

Michael Molnar (ChemE 1995), associate process engineering scientist, Dow Corning Corporation, was recently selected by the National Academy of Engineering (NAE) to participate at the 2015 China-America Frontiers of Engineering Symposium (CAFOE).

In Michael’s current role within Dow Corning Corporation, he supports multiple Dow Corning product lines in the areas of reaction engineering, process thermodynamics and flow sheet analysis, and pilot plant best practices for technology development. He is a recipient of two Dow Corning technical achievement awards and is a recognized inventor with seven granted patent families.

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