

# *Chemical Engineering at . . .*

## *Carnegie Mellon University*

LARRY BIEGLER

Carnegie Mellon University is located in Pittsburgh, Pennsylvania. Known as the Steel City and the City of Bridges, Pittsburgh is recognized internationally for its research and industry, cultural community, corporate headquarters, professional sports teams (Go Steelers! Go Penguins!) and the educational opportunities that more than 10 colleges and universities in the area provide. Carn-



*Carnegie Mellon University campus, located about 5 miles from the Golden Triangle of Pittsburgh.*

egie Mellon University was founded by industrialist and philanthropist Andrew Carnegie in 1900 as the Carnegie Technical Schools in Pittsburgh. In 1912, the schools became the Carnegie Institute of Technology, highly regarded in both the arts and technology. A merger in 1967 with Mellon Institute—the nation's first major private research institute—created Carnegie Mellon University. CMU consists of seven schools and colleges: Carnegie Institute of Technology, College of Fine Arts, Marianna Brown Dietrich College of Humanities and Social Sciences, H. John Heinz III College, Mellon College of Science, School of Computer Science, and the Tepper School of Business.

Carnegie Institute of Technology—Carnegie Mellon's College of Engineering—is one of the world's foremost engineering schools and is consistently ranked among the top 10 in the United States. CIT is the second smallest school among the Top 20 Engineering Colleges, which makes it especially well-suited for strong interdisciplinary research.

### HISTORY

The Department of Chemical Engineering was founded in 1905 and offered the degree through the School of Applied Science at the Carnegie Institute of Technology. At the time, the university educated primarily the children of steelworkers and other families in the Western Pennsylvania region. The first department head was Joseph James, who held that position until 1936.

Originally the department housed Carnegie Tech's activities in both chemical engineering and in chemistry. In 1936 the two disciplines diverged, and Warren McCabe became head of the Department of Chemical Engineering with a faculty of five. One of the first faculty members was Ernst Berl, a prominent German scientist who invented the Berl saddle—the packing rings used in distillation. Since then, the faculty,

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students, and alumni of the department have made numerous and significant contributions. The department has been the home to prominent chemical engineering academics, including Warren McCabe, Art Westerberg, Herb Toor, Ed Cussler, John Anderson, and Howard Brenner. Herb Toor and Ignacio Grossmann were named by AIChE in 2008 to the list of 100 chemical engineers of the modern era (post-WWII). Herb Toor became department head in 1965, and was appointed dean of Carnegie Institute of Technology (College of Engineering) in 1970. During his tenure he established the Department of Engineering and Public Policy and the Design Research Center, which seeded the current efforts in the process systems engineering area. These efforts were actively supported by Tom Fort and Art Westerberg, who succeeded Toor as department heads. John Anderson became department head in 1983 and was appointed dean in 1994. During his tenure as dean he established the Department of Biomedical Engineering. Ignacio Grossmann succeeded Anderson as department head and promoted the growth of the faculty. This was continued in 2004 by Andy Gellman, who succeeded Grossmann, and led a \$28M renovation of the research laboratories in Doherty Hall. Larry Biegler succeeded Gellman just last year.

The department has also included numerous leaders of industry and academia among its alumni, for instance: John Swearingen, former CEO of Amoco; Thomas McConomy, retired CEO of Calgon; Carol Dudley Williams, retired executive VP of Dow Chemical; Jonathan Rothberg, entrepreneur and scientist; Donna Blackmond, professor at Scripps; Chris Floudas, professor at Princeton; and Chris Macosko, professor at Minnesota.

The Department of Chemical Engineering is home to one of the strongest groups in complex fluids engineering. In process systems engineering it has pioneered the development of chemical process systems engineering and the use of computational tools for design optimization. More recent strengths include efforts in catalysis and surface science, in bioengineering, and in envirochemical engineering. Through-

out its history the department has managed to maintain an environment for students and faculty that is both scholarly and collegial.

## RESEARCH AREAS

### Biomolecular Engineering (BIO)

The Biomolecular Engineering group at Carnegie Mellon—Kris Dahl, Michael Domach, Todd Przybycien, James Schneider, Robert Tilton, and Kathryn Whitehead—has grown significantly over the past 15 years. Building on pioneering research in metabolic engineering by Mike Domach, the department has grown a diverse portfolio that includes upstream and downstream bioprocessing, protein- and nucleic acid-based drug delivery, bioanalytical chemistry, biosensing, and cellular/subcellular mechanics. Several factors have catalyzed this growth, the foremost being the highly collegial and collaborative environment within the department and the university, along with the proximity of the University of Pittsburgh School of Medicine and the West Penn Allegheny Health System and the establishment of the Department of Biomedical Engineering at Carnegie Mellon. The bio group's long-standing practice of encouraging the co-advising of student researchers and the sharing of expertise, techniques, and equipment culminated in a brick-and-mortar experiment in 2003: We renovated and co-occupied with Biomedical Engineering a large complex of open-format, shared labs in an off-campus building. The operational and programmatic success of this open, shared lab experiment—which can

be traced directly to our environment—formed the basis on which the chemical engineering research space in Doherty Hall was renovated in 2008 and on which the new biomedical engineering building (to open in 2015) was designed. We have leveraged Pittsburgh's position as one of the nation's leading centers for medical and life sciences research by participating in the joint Carnegie Mellon-University of Pittsburgh M.D.-Ph.D. training program since the mid-1980s, and by rolling out novel programs including a joint NIH biotechnology training grant program that had chemical and biomedical

DO YOU KNOW.....?	
These ChE authors:	<i>Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes</i> by Lorenz T. Biegler
	<i>Introduction to Biomedical Engineering</i> by Michael M. Domach
	<i>Systematic Methods of Chemical Process Design</i> by Lorenz T. Biegler, Ignacio E. Grossmann, Arthur W. Westerberg
	<i>Atmospheric Chemistry and Physics: From Air Pollution to Climate Change</i> by John H. Seinfeld, Spyros N. Pandis
These NSF Career Awards/ Presidential Early Career Award Recipients:	Shelley Anna and Kris Noel Dahl, the National Science Foundation Career Awards and John Kitchin, the Presidential Early Career Award for Scientists and Engineers
These members of the National Academy of Engineering:	Lorenz T. Biegler Ignacio E. Grossmann Krzysztof Matyjaszewski Jeffrey J. Siirola Arthur Westerberg
That the first annual AIChE meeting was held at Carnegie Technical Schools on Dec. 28-29, 1908, with four sessions, 13 papers, and an equipment exposition with eight exhibitors. Exactly 100 years later it was re-enacted in the same location by Dr. Dale Kearns, CMU alumnus and then-president of AIChE.	

engineering graduate students taking the full-year Foundations of Biomedical Sciences mega-course alongside first-year medical students. The parallel establishment and growth of the Department of Biomedical Engineering involved all of the bio faculty members of the Department of Chemical Engineering, as each has either a joint or a courtesy appointment with the Department of Biomedical Engineering and each has played key roles in the establishment of the educational, research, and administrative components of the new department. Here again the collegial, collaborative environment at Carnegie Mellon was decisive: The establishment of the Department of Biomedical Engineering was viewed as an opportunity for mutual growth in faculty and capability rather than as a divisive event.

Current major research efforts in the bio group include the design and synthesis of next-generation drug and gene delivery vehicles; the treatment of disorders related to subcellular mechanics; the design and development of scalable processes for the production of DNA vaccines and protein-based pharmaceuticals; the development of novel biosensing platforms for the rapid, selective detection of miRNA and other trace biomarkers; the improvement of the delivery of inhaled therapeutics by controlled surface transport; and determination of the molecular and cellular implications of exposure to nanomaterials. Collaborations with colleagues in the process systems engineering and complex fluids engineering clusters have led to the application of advanced optimization, computation, colloidal science, and interfacial science tools and approaches in these efforts.

### **Complex Fluids Engineering (CFE)**

The department has had a major research effort in colloid and interface science since the 1970s, stimulated in large part by interactions with Pittsburgh industry. The research effort is closely linked to Carnegie Mellon's innovative Master's degree and undergraduate minor programs in Colloids, Polymers, and Surfaces. Despite their centrality to so many of the products and materials that chemical engineers manufacture, few universities teach colloid or complex fluids engineering concepts at the undergraduate level. Often, the first task taken on by Carnegie Mellon researchers is to define a complex fluid for entering graduate students. Liquids that contain interacting dispersed particles ("colloids," which range in size from nanometers to micrometers), dissolved polymers, or surfactants are known as complex fluids. Their signature characteristic is an exquisite sensitivity of macroscopic properties, such as viscoelasticity or phase behavior, to strong intermolecular interactions among dispersed constituents in the fluid. These interactions often produce self-assembled "mesoscale" structures, such as micelles, in the bulk fluid or at the interface between the fluid and other materials. Complex fluid materials are engineered by manipulating those non-covalent intermolecular and surface forces. Products of complex fluids range from chemical mechanical planarization slurries to medicinal

lotions. Many solid materials such as ceramics or polymeric membranes are processed as complex fluids, and complex fluids often provide self-assembled templates to manufacture nanostructured materials.

Synergistic collaboration runs throughout the complex fluids engineering research effort. Faculty—Shelley Anna, Annette Jacobson, Aditya Khair, Meagan Mauter, Dennis Prieve, James Schneider, Paul Sides, Susana Steppan, Robert Tilton, and Lynn Walker—are working together currently to solve problems concerning the origin, control, and manifestations of electrical charge and electrostatic forces in low-dielectric constant liquids; the development of high-performance surfactants based on composite nanoparticles; the impact of non-Newtonian rheology on the electrokinetics of charged particles; the interfacial dynamics of dispersants deployed after oil spills; and the exploitation of surface-tension-driven flows to enhance pulmonary drug delivery. The research is not only highly collaborative but also highly multidisciplinary and benefits from thriving collaborations with the Chemistry and Physics Departments in the Mellon College of Science as well as the Biomedical Engineering, Civil and Environmental Engineering, and Materials Science and Engineering Departments in the College of Engineering.

### **Catalysis and Surface Science (CSS)**

The Catalysis and Surface Science group within the Department of Chemical Engineering comprises a wide range of research areas including catalytic properties of surfaces, enantioselectivity on chiral surfaces, sensor development, transport in porous solids, molecular simulation, and high-throughput methods of surface science. The group expertise includes both advanced experimental methods for materials characterization and synthesis as well as advanced theoretical and computational methods for simulation and understanding of novel solid properties. The group benefits from a well-equipped surface science laboratory.

The faculty—Andy Gellman, John Kitchin, Jim Miller, and Myung Jhon—have backgrounds and degrees in chemical engineering, chemistry, physics, and materials science, bringing an extremely diverse set of disciplines and expertise to the group. Their individual research groups include roughly 20 Ph.D. students and a few postdocs.

The interests in chemical reactions and catalysis of this group overlap strongly with the super-group Energy Science and Engineering, described later, largely based on a collaboration with the DOE National Energy Technology Laboratory in Pittsburgh. The focus of that work is catalytic processes for fossil fuel conversion, CO<sub>2</sub> activation and capture, and alloy development. Projects include the development of high-throughput catalytic reactor systems for rapid screening of alloy catalysts and optimization of catalytic alloy compositions.

Four other examples give an idea of the range of research being conducted. Numerous technological and materials

problems such as the effectiveness and stability of lubricants in magnetic-disk-drive technology must be solved. Myung Jhon participates in the Data Storage Systems Center, a former National Science Foundation Engineering Research Center devoted to the development of data storage technologies. Andy Gellman investigates the enantiospecific properties of chiral surfaces and chiral materials. Chiral molecules and surfaces exhibit “handedness.” Often the active form of a chiral pharmaceutical is only one of the possible enantiomers, and enantioselective chemical process must be developed to produce only that enantiomer. These issues are of critical importance for the synthesis of enantiomerically pure pharmaceuticals. John Kitchin is developing new computational methods for accurately and conveniently calculating the properties of oxides, with applications in materials design, chemical looping, catalysis, and electrochemical water splitting. Jim Miller and Andy Gellman are developing and applying high-throughput methods for study of alloy surface science across alloy composition space.

### **Envirochemical Engineering (ENV)**

The Envirochemical Engineering group includes faculty Neil Donahue, Spyros Pandis, and Meagan Mauter. Mauter collaborates with colleagues in Civil and Environmental Engineering and Engineering and Public Policy to address questions of water purification and policy. The Water and Energy Efficiency for the Environment (WE3) lab works to reduce the energy consumption of water desalination processes through material science and process design. Research is focused on re-defining the inputs of the water desalination process both by modifying the energy input—designing processes that use low-temperature heat in lieu of electricity—or by tailoring processes to work efficiently across a very low salinity or very high salinity feed streams. Current projects include a technoeconomic feasibility assessment of low-temperature heat driven separation processes, the development of novel capacitive deionization electrodes with drastically increased salt adsorption capacities, the characterization of biomacromolecular fouling on nanopatterned surfaces, and the development of novel membrane materials for membrane distillation processes.

The Center for Atmospheric Particle Studies is a highly collaborative research center including six faculty members, four with ChE affiliations. Director Peter Adams is a professor of civil and environmental engineering and engineering and public policy (EPP) with a courtesy appointment in ChE. Founding Director Neil Donahue is a professor of ChE, chemistry, and EPP. He currently directs the Steinbrenner Institute for Environmental Education and Research. Spyros Pandis is a research professor of ChE. Albert Presto is a research assistant professor of mechanical engineering (MechE) with a doctorate in ChE from CMU. Allen Robinson is head of the Department of Mechanical Engineering. Ryan Sullivan is an assistant professor of chemistry and MechE, and Satbir Singh

is an assistant teaching professor of MechE. Neil Donahue and Spyros Pandis are each cited more than 1,200 times per year in the peer-reviewed literature. Currently 25 students are conducting doctoral research in CAPS, including nine in ChE.

CAPS focuses on fine particles in the atmosphere for two reasons: these particles kill people and they constitute one of the largest uncertainties in climate science. This is also why there is a strong connection with policy research. Even though fine particles are present at very low levels—1 to 100 parts per billion by mass in air—they have a disproportionate effect because they can efficiently deliver concentrated material to critical locations. Two such locations are the human lung and nucleating water droplets in clouds. Inhalation of fine particles causes 50,000 premature deaths annually in the United States and millions worldwide. Particles also influence climate by scattering (and sometimes absorbing) light and by changing cloud properties—more particles scatter more light and also make clouds finer and whiter, thus the effect of particles on climate is mostly cooling. Much CAPS research focuses on understanding the life cycle of these particles and the different effects of different constituents in the particles.

Organic oxidation chemistry influences the formation and growth of ultrafine (< 30 nm diameter) particles to larger sizes. Spyros Pandis is the principal investigator on a project, PEGASOS, to use an instrumented zeppelin to sample particle production chemistry in the boundary layer over regions of Europe. Neil Donahue is heavily involved with a multinational CLOUD consortium at CERN in Geneva, Switzerland, to isolate the chemistry associated with new-particle formation (nucleation) in the atmosphere. Peter Adams has developed novel particle dynamics code that conserves number and mass during condensation and coagulation, and studies the influence of both new-particle formation and primary particle emissions on CCN budgets around the globe. Albert Presto, Allen Robinson, and Neil Donahue have focused on emissions from combustion sources, especially motor vehicles, showing that the organic material must be treated as being largely semi-volatile and that a significant amount of added pollution can arise from organics evaporated off of primary combustion particles as they dilute to ambient conditions.

### **Process Systems Engineering (PSE)**

Since the 1960s, Carnegie Mellon University has spearheaded the advancement of systems concepts to all areas of science and technology. Carnegie Mellon’s engineering faculty have been instrumental in catalyzing revolutionary changes resulting from the introduction of computer and systems technology to science and industry. In Process Systems Engineering (PSE), Carnegie Mellon’s effort began in the mid-’70s with the creation of the Design Research Center.

Research in PSE is currently directed by Larry Biegler, Chrysanthos Gounaris, Ignacio Grossmann, Nick Sahinidis, Jeffrey Siirola, and Erik Ydstie, while Art Westerberg is emeritus professor. The Carnegie Mellon PSE group represents the

largest one in the United States. The research is carried out in the department's state-of-the-art computational facilities by about 50 graduate students and 15 post-doctoral researchers and visitors, and is supported by funding in excess of \$3 million per year. The Center for Advanced Process Decision-making (CAPD), with more than 20 petroleum, chemicals, consumer products, and engineering companies, provides an umbrella organization for interactions with industry in the PSE area. Our research goal is to provide intellectual leadership in complex decision-making issues faced by process industries. Our underlying approach is based on developing and advancing systematic modeling and solution methods for multi-scale process systems engineering, covering the full spectrum from the molecular to the enterprise level.

The research work of the PSE group is focused in four major areas: optimization, design, operations, and control. Research in optimization includes theoretical and methodological advances in large-scale nonlinear programming, mixed-integer and disjunctive programming, global optimization, the optimization of differential-algebraic systems, stochastic programming, and machine learning techniques for the development of data-driven models and analytics. Topics in design involve applications in areas such as shale-gas facilities, biofuel plants, reaction/separation systems, energy and process water integration, process intensification, carbon-capture systems, fuel cells, solar cells and power systems, materials design (*e.g.*, catalysts, solvents, performance fluids), metabolic networks, and bioinformatics. Topics in operations include enterprise-wide optimization, supply chain management and optimization under uncertainty, planning and scheduling of batch and continuous process systems, real-time optimization, and electric power grids (smart grid). Finally, topics in control include adaptive control and on-line parameter estimation, self-learning control, control of distributed systems, thermodynamics-based control, passivity theory, the design and verification of process operating systems, and real-time data analysis.

Over the past two decades, the PSE group at Carnegie Mellon has graduated more than 150 Ph.D. students. Several of our students have taken academic positions at world-renowned institutions (*e.g.*, Georgia Tech, Imperial College, McMaster University, Northwestern University, Oxford University, Princeton University, Purdue University, University of Edinburgh, University of Illinois, and the University of Wisconsin) or have been employed by companies such as Aspen Technology, AT Kearney, Bank of America, British Petroleum, Chevron, Dow Chemical, ExxonMobil, IBM, McKinsey & Co., Royal Dutch Shell, OSIsoft, and United Technologies.

### **Energy Science and Engineering**

Energy-related research in chemical engineering at Carnegie Mellon has been the fastest growing segment of our research portfolio, covering many technologies including carbon capture and sequestration, electrochemical energy systems such as fuel cells, catalysis, solar photovoltaics,

environmental impacts of energy systems, and energy systems modeling and optimization. Faculty members working on these problems span the department's traditional disciplines and bring a wide range of expertise including catalytic surface science, applied electrochemical studies, materials science, computational molecular simulations, and the use of optimization and stochastic modeling techniques in systems research.

Much of the department's energy research is collaborative with the National Energy Technology Laboratory (NETL), a U.S. Department of Energy national laboratory, located in Pittsburgh and in Morgantown, WV. Carnegie Mellon University has partnered with NETL and four other universities to create the NETL-Regional University Alliance, which was founded in 2007 as the result of efforts led by Andy Gellman, who was head of our Department of Chemical Engineering at the time. The NETL-RUA fosters a research and development program that integrates researchers and activities from NETL and the five universities with the long term goal of transition of our energy infrastructure toward a sustainable system. It supports ~100 faculty members and ~150 Ph.D. students and postdocs with funding of ~\$20M/yr. The NETL-RUA has research activity in materials, process systems, catalysis, CO<sub>2</sub> management, sensors, energy conversion devices, gas hydrates, deep oil and gas, water management, combustion, shale gas development and conversion, and environmental impact of our energy infrastructure.

### **DOHERTY HALL RENOVATION**

Since 1908, the Department of Chemical Engineering has been housed in what was then called the School of Applied Sciences, one of the Carnegie Technical Schools. The building is located at the center of Carnegie Mellon's campus and is now named Doherty Hall in honor of Carnegie Mellon's third president. In early 2003 the department initiated planning of a major renovation of Doherty Hall, many portions of which had not been touched significantly for more than 50 years. The physical work on the building took place starting in the summer of 2006 and was completed by the end of 2008 at a total cost of ~\$28M. The result has been a major transformation of what had been a very old academic building into a truly modern facility that nonetheless retains its historic character.

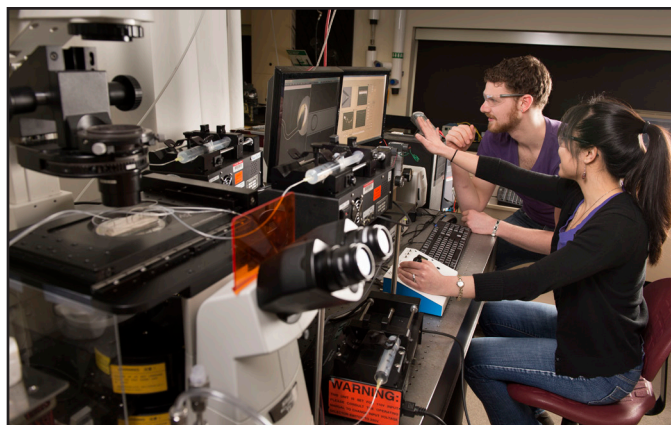
The entire ChE faculty was heavily engaged in all aspects of the design and planning of the renovation, with the result that five years after completion there have been no revelations of hindsight. In spite of the fact that the result was a paradigm shift in the operation of the department's research mission, thoughtful and careful planning precluded any subsequent regrets. During the course of determining the program and scope of the renovation, the faculty reached the decision to abolish the standard paradigm of assigning laboratories to individual faculty and research groups. Instead, large open laboratories and research offices were developed for each of the department's five major research areas: process systems



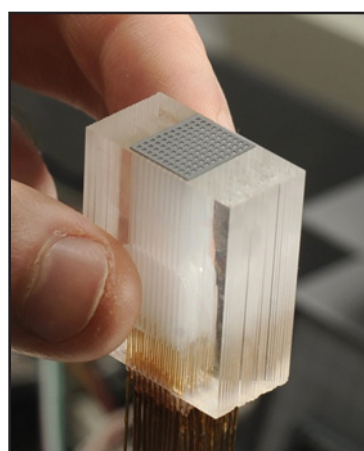
The Department of Chemical Engineering is housed in the recently renovated Doherty Hall on the CMU campus.

engineering; catalysis and surface science; bioengineering; complex fluids engineering; and envirochemical engineering. These large research suites are now shared by the groups in those research areas. The four major experimental laboratory suites consist of large open areas of 2,500 – 4,000 square feet outfitted with workbenches, hoods, and benches for instrumentation. Each also has smaller specialized rooms for functions such as cell culture, microscopy, and measurement tools that need to be isolated from the larger labs. Office space for those working in the labs is also shared by 10 – 20 researchers and is adjacent to but isolated from the laboratory space itself.

Since completion of the renovation, the ChE department has benefitted immensely from the many advantages of adopting a shared laboratory operating model. The elimination of walls and corridors effectively increases the usable space in the labs by ~30%. Space management and turnover is simplified by the fact that space is effectively assigned either to a researcher or to a piece of equipment, rather than being assigned to an individual faculty member's research group. When students graduate, their workspaces become available for assignment to



Grad students work in the Complex Fluids Engineering Lab.



A 10×10 multichannel microreactor array fabricated from glass in Prof. Andy Gellman's laboratory. The 100 reactors at the top of the glass reactor block are ~500 x 700 μm<sup>2</sup> in cross-sectional area. Each microreactor has its own reactant feed and product removal via the capillary glass tubes at the back of the reactor block. The multichannel reactor array is used in conjunction with composition spread alloy films (CSAFs) for high throughput studies of reaction kinetics on alloy catalysts with compositions spanning alloy composition space.

students in the incoming class. This allows individual research groups to fluctuate in size without affecting the effectiveness and efficiency of space use. The greatest beneficiaries of the shared space model are the students and researchers working in the laboratories. First and foremost, improvements in safety accrue from the fact that the likelihood of ever being alone in a lab is greatly diminished. Furthermore, students' research experience is enriched by the fact that they are aware of the work being done in related groups sharing the same lab. Collaborations arise simply because students are aware of instrumentation that would otherwise be hidden in a laboratory that they might never enter. Similarly, students doing computational modeling benefit from the fact that they share workspaces with related research groups.

The recent renovations to Doherty Hall have moved the departmental facilities into the 21st century. Furthermore, the investments in an open, collaborative community are obvious to visitors, potential hires, and student recruits alike. They have significantly improved the quality of professional life for the entire Carnegie Mellon chemical engineering community.



*The Department of Chemical Engineering's department heads, whose portraits adorn a wall in Doherty Hall, include: Joseph Hidy James, 1905-1936; Warren Lee McCabe, 1936-1947; Carl Corydon Monrad, 1947-1965; Herbert Lawrence Toor, 1965-1970; Robert Randle Rothfus, 1971-1973; Steven Louis Rosen (Acting), 1973-1973; Tomlinson Fort, Jr., 1973-1979; Arthur William Westerberg, 1980-1983; John Anderson, 1983-1994; Ignacio Grossmann, 1994-2002; Andrew Gellman, 2003-2013; and Lorenz Biegler, 2013-present.*

## CURRENT PROGRAMS

Our Chemical Engineering Department has a mid-size undergraduate program with more than 200 students in the sophomore through senior years and a graduating class of about 60-70 seniors; over half of our undergraduates are female. The department offers a B.S. in chemical engineering, and an integrated B.S./M.S. degree for undergraduates. The undergraduate curriculum is at once traditional and stable but flexible enough to accommodate built-in double majors, specialties, and minors. The curriculum emphasizes the acquisition of knowledge in basic science and mathematics during the first three semesters, acquisition and exercise of knowledge about engineering science in the next three semesters, and acquisition of knowledge and experience with engineering design, control, and operations in the final two semesters. The curriculum is especially flexible with concentrations, minors, and double majors that include biomedical engineering, public policy, business, and manufacturing operations. Our department has pioneered a unique educational program in colloids, polymers, and surfaces with a strong, dynamic laboratory component. Characteristics of the department's curriculum include a strong integrated set of process systems courses (unit operations, process design, product design,

process control, process optimization) that emphasize elements of decision-making as a key consequence of chemical engineering fundamentals. The objectives of the curriculum are to prepare students for employment, for graduate school, and to advance in their chosen careers. The undergraduate program also promotes strong exchange programs with other universities, including Imperial College in the UK, RWTH-Aachen, University of Dortmund in Germany, and EPFL in Switzerland; an exchange program with Yonsei University was also started in 2012.

Our Master's degree program has recently been restructured and expanded with a population of about 100 students. The program offers two options, a coursework-only degree (M.ChE.) designed to be completed in two academic semesters and a three-semester degree (M.S.) that involves both course and project work. Both degrees stress a core curriculum that prepares students for complex problems encountered in professional engineering practice. Emphasis is on developing a mastery of modern engineering concepts and tools beyond the undergraduate curriculum. These include proficiency in mathematical modeling and numerical methods for solving engineering problems such as computational fluid mechanics and transport, process simulation, and optimization, as well as

access to the leading-edge research programs. In addition, our department coordinates an interdisciplinary Master's degree in colloids, polymers, and surfaces (MCPS) that incorporates the science of nanoparticles, macromolecules, and interfaces, along with real-world applications including coatings and pigments, pharmaceuticals, surfactant-based products, cosmetics, pulp and paper, ink, food science, environmental science, agricultural products, polymers/advanced materials, and biomaterials.

Our Ph.D. program has grown steadily over the past two decades and has a population of about 90 Ph.D. candidates. It is supported by an external research budget of about \$9M/yr. and complemented by an additional 25 postdoctoral and visiting researchers. The Ph.D. curriculum includes first-year core courses designed to provide the student with a thorough knowledge of basic engineering science and advanced process analysis and systems. Courses beyond the first year cover advanced topics in specialized areas including surface chemistry and catalysis; thermodynamics; kinetic theory; process control; enterprise-wide optimization; process synthesis and optimization; applied mathematics; engineering design; computational chemistry and molecular simulation; electrochemical engineering, semiconductor processing, and polymeric materials; fermentation technology and biological process design; biomedical engineering; colloids and dispersions; and atmospheric chemistry. Our Ph.D. program is geared to students who want to join an elite global scientific and technological circle whose members have both the privilege and responsibility to shape the future. Balanced over the six research areas (BIO, CFE, CSS, ENV, PSE, ESE) and supported by a strong and vibrant graduate student organization (ChEGSA), our Ph.D. program is also an environment where students meet and form lifelong bonds with like-minded peers within their research group and across the program.

## NEW AND RECENT TRENDS

While the department continues to be strong in biomolecular engineering, catalysis and surface science, complex fluids, envirochemical engineering, and process systems engineering, it is also embarking into some new directions, most notably energy and sustainability.

Given the proximity of NETL (DOE's National Energy Technology Lab), the area of CO<sub>2</sub> capture has received considerable attention in the department. The research work in this area involves development of characterization methods for new CO<sub>2</sub> capture materials including sorbents, physical solvents, and chemical solvents. Recent work has focused on *in situ* Raman spectroscopy to characterize the physical solubility of CO<sub>2</sub> in solvents for pre-combustion capture applications, and the development of a microfluidic device to measure chemical absorption rates in solvents for post-combustion CO<sub>2</sub> capture applications. Research in this area has also involved development of efficient approaches for

modeling and optimization of large-scale PSA systems. These are based on fundamental advances in large-scale nonlinear programming algorithms, automatic differentiation for DAE systems, and reduced-order modeling for PDAE systems.

Another area receiving increased attention is shale gas, due to the location of Pittsburgh in the Marcellus shale gas play. Research in this area has involved the development of large-scale mixed-integer nonlinear programming models for the design of shale gas infrastructures for optimizing the number of wells to drill, size and location of new gas processing plants, section and length of pipelines for gathering raw gas, power of gas compressors, and planning of freshwater consumption for well drilling and fracturing. This research work has also involved an operational mixed-integer linear model to optimize life cycle water use for well pads. The objective of the model is to determine the fracturing schedule that minimizes costs for freshwater consumption, transportation, treatment, storage, and disposal. This effort promotes resource efficiency in water and energy systems by addressing technical and policy barriers to implementing utility-scale efficiency innovations; it is also complemented by assessment of environmental impact of shale gas production.

Another area that has received attention is air quality and climate change. An exemplary focus area has been the study of organic aerosols over longer timescales (minutes to hours) in the CMU smog chamber and in the CLOUD chamber at CERN, which allows one to observe and constrain secondary aerosol formation as well as the chemical processing of condensed-phase organics by gas-phase oxidants. Phase partitioning thermodynamics of low-volatility organic mixtures is also studied. The broad objective is to understand how oxidation mechanisms and their products, including ozone and aerosols, change with changing atmospheric composition.

The department continues to promote strong interactions with industry through centers such as the CAPD, which has more than 20 member companies in the areas of petroleum, chemical, engineering, and consumer products. Especially noteworthy is major funding that has been provided by the Dow Chemical Company (more than \$3.5 million over 5 years) in the CFE and PSE areas.

Finally, while the department continues to emphasize the teaching of chemical engineering fundamentals in the undergraduate and graduate programs, it is increasingly introducing advanced computational tools (including the Aspen Engineering Suite, COMSOL, GAMS, and gPROMS) throughout the curriculum.

## SUMMARY

In 1908, President Samuel Stadtler opened the first Annual AIChE Meeting with following words:

*"It is a matter of great pleasure to me that we were led to select this place for the first annual meeting of our*





*A gathering of students and researchers from the Carnegie Mellon University Department of Chemical Engineering's Center for Advanced Process Decision-making.*

*organization, because Pittsburgh<sup>1</sup> is now pre-eminently a chemical center, and therefore I feel that we will all be satisfied that we were fortunate in choosing this place ... this district has developed an enormous metallurgical industry, and you have also in this part of the country the magnificent electrical industry of Westinghouse and others, as well as the oil and the steel industries and all the connected branches, so that I feel that we have made no mistake in coming to Pittsburgh. I am particularly gratified, moreover, that we are welcomed in such a cordial manner by the Carnegie Technical Schools, because this is a typical example of the kind of institutions we would like to see developed in this country for the chemical engineering work we are trying to represent."*

Much has changed since then but the dynamic growth of chemical engineering and CMU's role remain strong. Carnegie Mellon University has had a thriving Chemical Engineering Department since 1905 with a long tradition of excellence, and pioneering research and service to chemical engineering. This has now evolved to a dynamic research department as well as a vibrant culture for undergraduate and graduate education.

Its current strengths include a well-balanced research program in BIO, CFE, CSS, ENV, ESE, and PSE as well as an innovative spirit that has led to unique research centers in complex fluids and process systems engineering.

Through strong connections to the Department of Energy and industry, spurred by the opportunities and challenges of new energy sources built over the past two decades, and rejuvenated through a major facility renovation, our department is poised to grow in the areas of energy and process systems, new materials, and atmospheric modeling toward an even brighter future.

## **ACKNOWLEDGMENTS**

Many thanks to Toni McIlltrot, Andy Gellman, Ignacio Grossmann, Todd Przybycien, Bob Tilton, John Kitchin, Neil Donahue, Meagan Mauter and Nick Sahinidis for their significant contributions to this article. □

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<sup>1</sup> Pittsburgh's current spelling was not resolved until 1911.