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CHEMICAL ENGINEERING
The Department of Chemical Engineering at Carnegie Mellon University invites you to learn about its faculty, areas of research, facilities, research centers, graduate programs and graduate student life. ChemE at CMU originated over a century ago from the School of Applied Sciences within the Carnegie Technical Schools. The Technical Schools evolved into Carnegie Mellon University and the Department of Chemical Engineering issued from the School of Applied Sciences; both are now internationally respected centers of knowledge and research. ChemE at CMU has been home to major names in chemical engineering such as McCabe, Berl, Toor, Brenner and Westerberg.

Today, ChemE has a faculty of 22 internationally known professors, some holding joint appointments with other departments. On average, ChemE awards approximately 60 B.S., 20 M.S. and 15 Ph.D. degrees each year. The department’s research interests fall into six basic groups: Bioengineering, Catalysis and Surface Science, Complex Fluids Engineering, Envirochemical Engineering, Process Systems Engineering and Energy Science and Engineering. The Process Systems group with four outstanding faculty is one of the strongest of its kind, if not the strongest, anywhere. Also, ChemE at CMU has been known over decades for its strength in colloid and polymer science. The other groups have emerged over the last twenty five years. We have formed the super-group called Energy Science and Engineering to focus attention on the depth and breadth of ChemE’s engagement with a leading challenge of our time. These research collectives and their associated faculty are the principal focus of this brochure.

ChemE’s home at Carnegie Mellon is Doherty Hall, a historic building at the center of campus. Renovated in 2008/9, the research space is unique in its philosophy of large multi-faculty spaces where the strong community and collegiality in the department find their full expression, fostering creativity in its research. We hope this brochure helps you get to know ChemE at CMU. For more details and the latest information, please visit www.cheme.cmu.edu.
RESEARCH AREAS

The Department of Chemical Engineering at Carnegie Mellon hosts a wide variety of research programs, including some of the strongest anywhere. The department’s many research projects are grouped by facilities, shared interests, and shared laboratories into the following areas:

BIO - Bioengineering
CSS - Catalysis and Surface Science
CFE - Complex Fluids Engineering
ENV - Environchemical Engineering
PSE - Process Systems Engineering
ESE - Energy Science and Engineering

A general description of each of these research areas appears in the following pages. These groups reflect both traditional and evolving areas of interest in the department. The matrix below maps our self-organization into more common topics. Many of the faculty have activities in more than one area and many of the faculty also have appointments in other departments. As apparent from the table, the classical topics of chemical engineering are embedded in our groups.

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Biotechnology and biomolecular engineering are important areas in the Department of Chemical Engineering. The faculty focus on metabolic engineering, the production, processing and delivery of nucleic acids, proteins and vaccines, bioanalytical technologies and the mechanics, structure and function of the cell nucleus. In these areas, faculty apply principles of fundamental biology, biophysics and physical chemistry in addition to traditional chemical engineering concepts of transport phenomena, kinetics, thermodynamics, colloid and interfacial science and modeling.

The faculty have created novel optical and spectroscopic tools to probe the structure and function of proteins at interfaces, such as those presented by chromatographic media, and to assess the propensity of proteins to crystallize under pharmaceutical processing conditions. Novel affinity ligands, including surfactants that hybridize to specific DNA targets for chromatographic purification, are also under development. Quantitative imaging methods, including nuclear magnetic resonance, fluorescence, and nanoscale mechanical measurements, are brought to bear on intact cells and organelles to better understand metabolic pathways, stem cell differentiation, the progression of cancer, and diseases of the nuclear lamina. Robotic technologies for cell proliferation and drug discovery studies are being explored in collaboration with the Robotics Institute; highly adaptable biosensors, rapid DNA sequencing platforms and micro-scale cell sorting schemes are under development.

Other chemical engineering faculty also have significant efforts in bioengineering and biotechnology. Nick Sahinidis develops practical algorithms for protein structural alignment. Ignacio Grossmann analyzes metabolic flux optimization and product development for pharmaceuticals.

Bioengineering students have the opportunity to participate in a formal Ph.D. Training Program in BioProcess Engineering & Design that integrates bioengineering coursework with basic biology coursework from the University of Pittsburgh’s School of Medicine. This unique training program educates bioengineers who are freely conversant with biologists and clinicians. Bioengineering faculty and students also maintain close interactions with Carnegie Mellon’s Department of Biomedical Engineering, where research expertise is found in biomechanics, tissue engineering, regenerative medicine, cellular and molecular biotechnology, bioimaging and bioinformatics.

### Participating Faculty

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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, sensor development, transport in porous solids, molecular simulation, and frictional properties of solid-solid interfaces systems. 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 described later in this brochure.

The faculty have backgrounds and degrees in chemical engineering, chemistry, physics and mathematics, bringing an extremely diverse set of disciplines and expertise to the group. Their individual research groups include roughly 20 graduate students and half a dozen postdocs.

The interests in chemical reaction catalysis of this group overlap strongly with the Energy Science and Engineering super-group described later, largely based on a collaboration with the DOE National Energy Technology Laboratory located in Pittsburgh. The focus of that work is catalytic processes for fossil fuel conversion and for CO₂ activation and capture. Projects include the development of high throughput catalytic reactor systems for rapid screening of alloy catalysts and optimization of catalytic alloy compositions. A second direction is the capture of CO₂ by sorbents.

Three 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 molecule is only one of the two possibilities. These issues are of critical importance for the synthesis of enantiomerically pure pharmaceuticals. John Kitchin is embarking on a five year research grant aimed at improving electrocatalysis for the oxygen evolution that accompanies hydrogen production.
Interfacially dominated materials and fluid processing technologies are invariably characterized by molecular and compositional complexity. Many important materials are colloidal, which means they are multi-phase mixtures having macroscopic properties dominated by long-range interactions between distinct physical structures in the nanometer to micrometer size range. Pharmaceutical suspensions, low volatile-organic-content coatings, agricultural emulsions, ceramic precursors and electrophoretic display media are just a few examples.

One must understand and control physical forces on the nanometer scale in processes involving complex fluids. Phenomena at the nanometer scale (e.g., self-assembly of surfactants and polymers in solution or on the surfaces of dispersed particles, solvent and solute ordering near interfaces) control phenomena that occur at the micrometer scale (e.g., nucleation of multi-particle aggregates, formation of thin fluid films). These phenomena in turn are embedded in effects at the macroscopic scale (e.g., viscoelastic flows, phase separation, coating flows).

The goal of the Complex Fluids Engineering group is to discover and use the links among the nano-, micro- and macro-scales in order to more effectively engineer myriad fluid processing technologies. This group is uniquely positioned to address the higher level complexities that are introduced by strongly interacting solutes in multi-component mixtures.

Students in the Complex Fluids Engineering group enjoy a highly collaborative research and educational environment. It is common for students to be co-advised by two faculty members with complementary expertise, or to work as part of a dynamic team of students having different research advisors who join forces to solve interdisciplinary research problems. The Complex Fluids group uses the well-equipped, multiuser PPG Industries Colloids, Polymers and Surfaces Laboratory, and shares the specialized instrumentation maintained by individual faculty groups.

The Complex Fluids Engineering group has a rich tradition at CMU. Students are currently exploiting a wide variety of experimental and theoretical techniques to investigate, for example, supramolecular engineering of interface structure via polymer/surfactant complexation and co-adsorption, colloidal forces and aggregation dynamics, electrophoretic deposition of colloidal crystalline arrays for display technologies, functionalized lipids for drug delivery and DNA separation, shear-induced structural transitions in self-assembling liquids, and the rheology of dense suspensions.
Emissions of gases and particles by industrial and other anthropogenic sources results in increased levels of a variety of atmospheric pollutants. The faculty focus on understanding of atmospheric pollution and on developing the tools needed to reduce potentially harmful constituents in the air. Using an integrated approach to solve air quality problems, they consider source emissions, atmospheric transport and chemistry, and the ultimate removal of the pollutants from the atmosphere by deposition. The group is currently working on problems ranging from smog formation in large urban centers to global climate change. Peter Adams from Civil and Environmental and Allen Robinson from Mechanical Engineering join the ChemE faculty to form a robust core of engineers working on environmental issues.

Research includes the development of detailed state-of-the-art computer models describing various components of the atmospheric system as pollutants move from sources to receptors, as well as carefully controlled laboratory studies of fundamental processes related to the formation of pollutants and their properties. The new Carnegie Mellon Air Quality Laboratory, located in the Chemical Engineering Department, is a state-of-the-art facility including a clean room, two indoor smog chambers, and two mobile air sampling laboratories. Additional resources include a wind tunnel and a source-testing laboratory. The air quality program also includes field studies at locations ranging from congested urban centers to remote areas of the world.

Airborne particulate matter (PM) poses serious health risks to susceptible members of the U.S. population and to sensitive ecosystems. The lack of understanding of the PM-health effects links limits the design of cost-effective PM control strategies. A paucity of physiological data, the difficulty of establishing the PM source-receptor relationships and the shortcomings of existing instrumentation for PM measurements complicate the design problem. The CMU Air Quality team, with funding by EPA and DOE, has established a PM research center for the comprehensive multidisciplinary study of the above issues. The center includes investigators from 12 universities, two national laboratories and a number of private companies.

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The goal of the Process Systems Engineering group is to provide intellectual leadership in complex design and operation issues faced by process industries. The underlying approach is based on developing and advancing systematic modeling and solution methods for the optimization and control of multi-scale process systems, ranging from molecular level to the enterprise level. Specifically, the PSE group focuses on the optimization and control of process, energy and biological systems. Topics covered include nonlinear, mixed-integer and disjunctive programming; global optimization and stochastic programming; optimization of differential algebraic systems; synthesis of separation (distillation, PSA), energy (solar, fuel cells, IGCC) and water systems, and molecular design; planning, scheduling and enterprise-wide optimization (batch and continuous processes); optimization methods for data-handling problems; adaptive, self-learning and nonlinear control; passivity theory; systems biology (biomolecular design and metabolic networks).

The PSE faculty authored a textbook on process design (Systematic Methods of Chemical Process Design); many academic departments have adopted research strategies developed at Carnegie Mellon. Recently Prof. Biegler authored a book Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Processes published by SIAM. The PSE faculty play important editorial roles for a number of journals, including AIChE Journal, Automatica, Computational Management Science, Journal of Global Optimization, Computers and Chemical Engineering, Optimization in Engineering, I&EC Research, Optimization Letters, Optimization Methods and Software and SIAM Journal on Optimization. The group’s research activities include numerous international interactions and research collaborations.

The research in the PSE area is carried out by approximately 25 graduate students and 10 researchers within the department’s Center for Advanced Process Decision-making (CAPD), and with funding over $2 million per year. The CAPD provides an umbrella organization for interactions with industry in the Process Systems Engineering area. Based on fundamental research in modeling, optimization and control, the CAPD addresses a wide range of applications in product and process design, process control and enterprise-wide optimization. These applications are addressed through methodologies that are based on process modeling (dynamics, superstructures), mathematical programming (nonlinear and mixed-integer programming) and modern search methods (logic-based).

See also the Center for Advanced Process Decision-making (CAPD) on page 39.
Energy-related research in ChemE at CMU has been the fastest growing segment of our research portfolio. Energy research spans many technologies including CO$_2$ capture and sequestration, electrochemical energy systems such as fuel cells, catalysis, solar cell production, energy system modeling, scheduling and optimization. A wide range of approaches are used such as computational molecular simulations and model single crystal surface studies, applied electrochemical studies, materials preparation, computational molecular simulations and optimization and stochastic modeling techniques in systems research. More than half the faculty in ChemE are involved. Reflecting the volume of energy research and the cross-cutting range of energy-related work, the department has recognized a new grouping of faculty now called Energy Science and Engineering.

Much of the department’s energy research is collaborative with the National Energy Technology Laboratory (NETL), a Department of Energy national laboratory. Carnegie Mellon University has joined forces with NETL and four other universities to create the Regional University Alliance run by Andy Gellman. NETL/RUA fosters a research and development program that will move energy infrastructure toward a sustainable state. It supports ~100 faculty members and ~150 Ph.D. students and postdocs with funding of ~$20M /yr. The NETL/RUA has interests in materials, process systems, catalysis, CO$_2$ management, sensors, energy conversion devices, gas hydrates, deep oil and gas, water management and combustion.
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<td>B. Erik Ydstie</td>
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Shelley L. Anna
ASSOCIATE PROFESSOR OF CHEMICAL ENGINEERING, MECHANICAL ENGINEERING AND PHYSICS (COURTESY)

Recognition
National Science Foundation CAREER Award
Achievement Award, Solutia, Inc., Springfield, Massachusetts

Publications

Professor Anna develops novel methods to synthesize soft materials precisely and to characterize physical mechanisms governing their dynamics. Her research group uses experiments in fluid dynamics combined with physical modeling and analysis.

Soft materials are critical to numerous engineering technologies from consumer products and pharmaceuticals to optical devices and energy solutions. Common to all soft materials is the presence of an underlying structure, whether droplets, defects or macromolecules. Microfluidics has revolutionized synthesis and characterization of soft materials by enabling precise fabrication and control of flows at length scales that interact with the microstructure.

Professor Anna’s research group generates monodisperse emulsion droplets micrometers to nanometers in size. She has developed a technology for producing submicron droplets using a fluid mechanical phenomenon called tipstreaming. Collaborating with Prof. Walker, Prof. Anna uses tipstreaming to create nanoscale droplet reactors to synthesize transition metal nanoparticles. The particles can be used for accurate cancer detection and targeted therapies. Other ongoing projects include investigations of coalescence of droplets on surfaces for spray cooling, inkjet printing and fuel cell applications; and use of microscale methods for characterizing sorption kinetics at fluid interfaces.

Microscopic defects strongly affect the flow behavior of liquid crystals and concentrated surfactant solutions. Defects are important in optoelectronic devices and displays and the processing of coatings, adhesives and biomaterials to encapsulate drugs. Neither theory nor experiment is adequately developed, however, to describe the fluid dynamics near defects quantitatively. Prof. Anna’s research bridges this gap by using microfluidic devices to generate idealized arrays of microscopic defects, and by characterizing the evolution of the defect microstructure and the fluid stresses when defects are subject to well-defined flows.

Fluid invasion into saturated porous media is central to several key technologies for energy and the environment, including carbon sequestration, aquifer remediation and oil recovery. The fluid mechanics of invasion controls the efficiency and efficacy of a given technology. In collaboration with Prof. M. Ferer (WVU) and the National Energy Technology Laboratory (NETL), Prof. Anna’s research group has developed model microfluidic networks to characterize the pore-level dynamics of invasion to inform and validate pore level simulations.

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www.cheme.cmu.edu/people/faculty/sanna.htm
Lorenz T. Biegler
BAYER PROFESSOR OF CHEMICAL ENGINEERING, UNIVERSITY PROFESSOR

Professor Biegler’s research projects center on the development and application of concepts, algorithms and applications of optimization and numerical methods for process design, analysis, operations and control.

**Advanced algorithms for flowsheet simulation, optimization and sensitivity analysis.** The focus is on the development of numerical methods for simulation and optimization of challenging process applications. This work includes the development of interior point and active set algorithms for nonlinear programming and nonlinear complementarity problems, as well as efficient decomposition strategies for these problems. These algorithms form the core solvers for many areas in process design, control and operations. Emphasis is on efficient methods for large-scale optimization problems that arise in chemical engineering applications and energy systems.

**Development of large-scale nonlinear programming methods for optimization of systems of differential and algebraic equations (DAEs).** Projects include analysis of stability and accuracy for approximate DAE solutions, algorithms for optimal control problems and methods for large-scale nonlinear programming. These problem types are addressed through large-scale nonlinear programming formulations that can be solved efficiently for large-scale systems. Applications include batch processes, fuel cells, complex dynamic separations, biological fermentations and polymerization reactors.

**Real-time algorithms for nonlinear estimation, control and optimization.** These methods include the application of maximum likelihood and optimization concepts for parameter estimation, data reconciliation and gross error detection for steady and dynamic problems. In addition, based on fast sensitivity-based decompositions, efficient optimization strategies are being implemented for nonlinear control and real-time optimization, and demonstrated on large-scale chemical and energy processes.

**Design and optimization of processes based on detailed PDE-based models.** Optimization applications include periodic adsorption processes such as pressure swing adsorption, simulated moving beds, complex, multiphase reactors and computational fluid dynamics models that are spatially distributed and may also have dynamics components. Challenging applications arise in CO₂ capture and energy network and production systems.

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**Recognition**
Olaf A. Hougen Visiting Professorship, University of Wisconsin, 2009
Warren K. Lewis Award for Chemical Engineering Education, AIChE, 2009
INFORMS Computing Society Prize, October, 2009
CACHE Computing in Chemical Engineering Award, American Society for Engineering Education, 2007
Fulbright Senior Research Fellow, Universität Heidelberg, Germany, Fall, 2006
Computing in Chemical Engineering Award, CAST Division, AIChE, 2000

**Publications**
Professor Dahl uses rheological, biophysical and optical techniques to understand the structure and organization of the cell nucleus.

**Diseases of the nuclear lamina.** Many diseases result from the loss or mutation of lamins and other structural proteins at the nuclear envelope and in the nuclear interior. Prof. Dahl’s studies compare normal cells with cells in which structural proteins are either chronically absent or rapidly down-regulated (as by RNAi-mediated gene silencing). These studies reveal the adaptations made by nuclei to altered mechanostuctural environments in order to restore function.

**Stem cell differentiation and cancer progression.** Nuclear shape and chromosome positioning change dramatically during stem cell differentiation and cancer progression. Fluorescence techniques are being combined with quantitative biophysics to track recruitment of transcription factors or cell cycle regulators to differentiation specific or cancer-specific genes while cells or nuclei are under well-defined imposed forces.

**Mechanotransduction.** Mechanotransduction allows cells to sense mechanical forces and adapt by changing gene expression. In 2010 Prof. Dahl received an NSF CAREER Award to work on the hypothesis that mechanical force reorganizes the nucleus and thereby regulates gene expression.

HeLa cells overexpressing GFP-spectrin and labeled for emerin (red) and DNA (blue) show enhanced spectrin at the nuclear envelope. Nucleoskeletal spectrins are responsible for a balance of mechanical forces and resilience after deformation.

Kris N. Dahl
ASSISTANT PROFESSOR OF CHEMICAL ENGINEERING AND BIOMEDICAL ENGINEERING

**Recognition**
National Science Foundation CAREER Award
Young Investigator Award Gold from the World Congress of Biomechanics
Ruth L. Kirchstein National Research Service Award: Post-doctoral research fellowship from NIH

**Publications**
Professor Domach studies fundamental and applied aspects of biomedical engineering and cell biology. He concentrates on cellular processes, cell physiology/energetics, enzymology and novel biomedical devices.

Parallel Experimentation Systems for Drug Discovery and Cell Development.
A collaboration with a nearby medical research group aims to develop an automated system for performing 100 or more cell growth experiments in parallel. A unique facet is when cells present certain cues that are detected via optics or fluorescent probes, the abiotic environment can be altered by robotic devices so that cellular control mechanisms can be directed or tested in detail. One current application entails expanding stem cell populations for engraftment into patients. Another project involved building arrays of surface sensors to track the location and proliferation of hundreds of cells.

Cellular Processes. The goal is to understand the behavior of cells in bioreactors and, thus, reactor performance in terms of biochemical reaction and control mechanisms. Current work entails developing in situ NMR and fluorescent spectroscopic methods for observing intracellular reaction processes. Coupling the experimental investigations to mathematical model development also is a key component of this work.

Environmental Metabolism.
The kinetics of polycyclic aromatic hydrocarbon degradation are under investigation. Prof. Domach uses fluorescence spectroscopy to observe the fate of hydrocarbons in intact, model soil-water systems.

Network representation for computer-aided prediction for optimal metabolic flux distribution for therapeutic DNA production.
Research in Professor Donahue's laboratory focuses on three interrelated topics: the oxidation pathways of reduced compounds throughout the atmosphere, measurement of atmospheric compounds, including free radicals and stable molecules, and the fundamental quantum mechanics and dynamics controlling reactivity and causing variation in reactivity among related chemical systems.

**Atmospheric Oxidation Mechanisms.** Reduced compounds react in the atmosphere with oxidants including hydroxyl (OH), ozone (O₃) and nitrate (NO₃). Their oxidation products include oxygenated organics (aldehydes, ketones, organic acids, carbon monoxide, and carbon dioxide), ozone, and organic aerosols. Prof. Donahue's students observe the mechanisms connecting these reactants and products by initiating the oxidation in a flow-tube and observing the reaction downstream. The time scale of these experiments permits observation of mechanisms step-by-step while studying interactions typical of the real atmosphere. This chemistry in the CMU smog chamber occurs over longer timescales (minutes to hours), allowing observation and constrain of secondary aerosol formation as well as the chemical processing of condensed-phase organics by gas-phase oxidants. The broad objective is to understand how oxidation mechanisms and their products, including ozone and aerosols, change with changing atmospheric composition.

**Fundamental Reactivity.** Chemical reactivity can evolve dramatically among a series of related reactions. Reactivity can differ by a factor of a million or more, and similar reactions can have qualitatively different reaction products. This has profound consequences for atmospheric chemistry, combustion, and all other systems involving complex mechanisms. It also indicates that observation without fundamental understanding is dangerous. A major objective of our work is to understand the fundamental quantum mechanics and reaction dynamics describing this evolution.

**Organic Phase Partitioning.** We are developing methods to treat the coupled oxidation chemistry and mixing thermodynamics that control the levels and properties of organic particulate matter in Earth's atmosphere. Organic aerosol consists of millions of individual compounds, many of them uncharacterized, but we are able to identify key bulk properties of the particulate organic phase and then describe the solution thermodynamics in terms of these measurable properties.
Professor Gellman’s group uses a wide variety of experimental methods to study surface chemical processes such as the bonding of molecules to metal surfaces, surface structure, reaction kinetics, adsorption and catalysis.

The use of ultra-high vacuum surface science methods to create and study well-defined catalytic surfaces allows Prof. Gellman’s group to investigate problems in heterogeneous catalysis at the most fundamental level. One of his primary focus areas is enantioselective chemistry of chiral metal surfaces. Because most pharmaceuticals are chiral, enantioselective chemical processing is the key challenge to preparation of the vast majority of pharmaceuticals. Prof. Gellman was the first to realize that some single crystal metal surfaces can be chiral in spite of the fact that the bulk structures of metals are highly symmetric and, therefore, achiral. His group has pioneered the effort worldwide to study and understand enantioselectivity on naturally chiral metal surfaces.

Recent efforts in Prof. Gellman’s group have been focused on the development and application of high throughput tools for the study of surface and materials science. These will rapidly accelerate the study of alloy surface chemistry and structure sensitive surface chemistry. His group has developed tools for the preparation and characterization of Composition Spread Alloy Films (CSAFs) which contain all possible compositions of alloys such as Pd$_x$Cu$_y$Au$_{1-x-y}$ (Figure). Spatially resolved measurement of their catalytic properties allows parallel collection and study of the catalytic activity of ternary alloys of all possible compositions. His group is also developing the use of Surface Structure Spread Single Crystals (S$^4$Cs) which expose single crystal surfaces of all possible orientations on one sample. These methods will increase by a couple of orders of magnitude the rate at which one can study alloy composition and surface structure effects on catalytic surface chemistry.

Top panels. Composition distribution across a Pd$_x$Cu$_y$Au$_{1-x-y}$ CSAF. Bright regions indicate high concentrations of the relevant component. Lower panel. Variation in the rate of HD production from H$_2$-D$_2$ exchange across the Pd$_x$Cu$_y$Au$_{1-x-y}$ CSAF. Cu and Au both retard the rate of HD exchange but the effect is nonlinear in Cu concentration.

Andrew J. Gellman
HEAD OF CHEMICAL ENGINEERING AND LORD PROFESSOR OF CHEMICAL ENGINEERING, CHEMISTRY (COURTESY), MATERIALS SCIENCE AND ENGINEERING (COURTESY)

Recognition
Ipatieff Prize, American Chemical Society, 1998
Alfred P. Sloan Research Fellow, A.P. Sloan Foundation 1991-1993

Publications

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The goal of Professor Grossmann’s work is to develop novel mathematical programming models and techniques for a variety of problems in process systems engineering.

Logic-based and Global Optimization
New modeling and solution methods are being developed for linear and nonlinear discrete-continuous optimization problems. These are based on generalized disjunctive programming (GDP) in which equations and symbolic logic relations are formulated as part of the optimization problem. Based on recent connections with disjunctive programming theory by Balas, new reformulations for both linear and nonlinear GDP problems based on hull relaxations are being investigated that exhibit tighter relaxations. Global optimization techniques are also being investigated that exploit the mathematical structure of disjunctions involving nonconvex functions, particularly bilinear and concave functions. Special vector cuts for bilinearities in process network problems are also being investigated.

Optimization of Water, Energy and Process Systems
Models and solution techniques based on mixed-integer nonlinear programming are being developed for the synthesis of integrated process water networks, design of biofuel plants (corn and lignocellulosic bioethanol and biodiesel) and for the optimal synthesis of IGCC plants. For the synthesis of integrated water systems, effective global optimization techniques are being investigated. These in turn are being incorporated in a novel model for simultaneous optimization with heat integration and water integration for the synthesis of process flowsheets, particularly for biofuel plants.

Planning, Scheduling and Enterprise-wide Optimization
Mixed-integer and disjunctive optimization models and solution techniques are being developed for the planning and scheduling of batch and continuous process systems, and for supply chain optimization problems that arise in the process industry. Major applications include design and planning of offshore oil and gas field facilities under uncertainty, planning of oil refineries, crude oil scheduling and multisite capacity planning problems of air separation plants. Stochastic inventory models are also incorporated in supply chain optimization problems, while uncertainties are addressed through multistage stochastic programming techniques.

Decomposition methods based on Lagrangean and two-level decomposition with aggregate models are being investigated to effectively solve these large-scale optimization problems.
Annette Moff Jacobson
TEACHING PROFESSOR OF CHEMICAL ENGINEERING, DIRECTOR COLLOIDS, POLYMERS AND SURFACES PROGRAM
ASSOCIATE DEAN OF UNDERGRADUATE STUDIES

Surfactant micellization, solubilization and adsorption phenomena; polymer and colloid characterization.

Solubilization Phenomena
Solubilization is the incorporation of compounds into the aqueous phase in excess of their water solubility, accomplished through the formation of aqueous micelles of surfactant. Current work includes application of capillary electrophoresis using micellar species as a materials separation method.

Colloid and Polymer Characterization
Determination of electrophoretic mobility of colloidal contaminants in water is useful in water treatment processing. Recent research shows that electrophoretic property measurement is important in determining the quality of the treatment process, indicating whether additional treatment is required.

Research in polymers includes characterization methods for applications that include polymeric nanofibers and suspension polymerization processes.

Colloids, Polymers and Surfaces (CPS) Program
Professor Jacobson is Director of the CPS Program, an interdisciplinary educational program providing coursework and an M.S. degree in the study and applications of nanoparticles, macromolecules, interfaces and the complex fluids formed by these materials. The program includes the PPG Industries CPS Laboratory, a facility used for teaching and research for graduate and undergraduate students.

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Recognition
Academic Advising Award, Carnegie Mellon University, 2003

Publications


Focusing on the fundamentals in engineering science and their application to the state-of-the-art engineering problems, Professor Jhon is primarily involved with the mathematical modeling of complex engineering systems using finite element, Monte Carlo, and molecular dynamics simulations. In addition, the Lattice Boltzmann method is currently being implemented via parallel computing schemes to examine multi-scale and multi-phenomena complex engineering systems.

Prof. Jhon has also synthesized and characterized many different polymeric systems including polyaniline to make electrorheological (ER) fluids, consisting of a suspension of micron-sized particles in a nonconducting fluid, which plays an important role in electromechanical control devices. He constructed a universal scaling function for the ER yield stress over a broad range of electrical field strengths, by hybridizing both the polarization and conductivity models. He also examined rheological properties of complex fluid systems including perfluoropolymers, polymer/clay nanocomposites, and polymer/carbon nanotube composites.

Prof. Jhon is investigating mechanical and reliability issues in information storage devices at the Data Storage Systems Center (DSSC). Mathematical software suitable for designing next-generation drives, including heat assisted magnetic recording, is being developed in collaboration with industrial partners at the DSSC.

Transport processes of lubricant film in nanoscale confined geometries are being examined. Experimental and theoretical investigations in nanotribology, nanorheology and microstructural analysis are also under way. In conjunction with the Institute for Complex Engineered Systems (ICES), he is pioneering the modeling of nanoscale devices which is extremely important in electronics packaging area and next-generation silicon-on-insulator transistors as well as the design of the direct methanol and hydrogen fuel cells. He is also exploring the manufacturing and development of deposition equipment for organic light-emitting devices (OLEDs), which is one of the rapidly growing display technologies as well as chemical mechanical planarization (CMP) equipment, which is extensively used in the semiconductor devices manufacturing industry. He has been converging these technologies via virtues of nanotechnology, which will have a great impact in the nanomanufacturing area.

Prof. Jhon recently developed new research projects on nano-convergent technologies that are critically important to human interface systems (e.g., silicon-based flexible display, light-emitting devices and sensors). In addition, he is involved with policy-making on nanotechnology, green energy and remanufacturing areas.
Professor Khair’s research lies in modeling micro- and nano-scale transport and fluid flow, which plays a significant role in microfluidics, self assembly, and complex fluids. Being particularly interested in electrically driven, or electrokinetic phenomena, Prof. Khair investigates electrokinetic flows in nanochannels having dimensions comparable to the length scale of the electrical double layer, thereby enabling geometric ‘engineering’ of nano-scale electrostatic interactions for sample pre-concentration, energy harvesting, and single molecule studies. A second theme of research is complex fluids, materials whose rheology lies between fluids and solids. Prof. Khair proposes to “design” rheological properties via tuning of nano-scale interparticle forces. Prof. Khair will study the nonlinear electrophoresis and self-assembly of charged colloidal dispersions.

Prof. Khair also is interested in the fundamental physics of concentrated electrolytes and ionic liquids near highly-charged and nano-structured surfaces, including the role of steric repulsion and electrostatic correlations between ions, and fluid flow within the electric double layer. These effects are relevant to nano-scale manipulation of fluids and particles and the rational design of energy storage devices.

The steady-state salt concentration established due to an electric field applied parallel to a periodically-varying surface charge, under strong fluid flow (black arrows). Notice how the strong flow focuses the salt into a “jet” of high concentration (red).
Professor Kitchin’s research group focuses on energy and environmental applications of electrochemistry and on computational methods for studying chemical reactions at catalyst surfaces. He investigates CO₂ capture, electrochemistry, fuel cells, and multiscale ab initio modeling of heterogeneous catalysis.

Prof. Kitchin investigates solid sorbents and electrochemical processes as methods for capturing CO₂ from the exhaust gas in a power plant. His group modifies the porous cathodes of solid oxide fuel cells with high surface area infiltrants to increase the efficiency of the fuel cell. These same synthesis methods are being used to create new, mixed-metal oxide electrocatalysts for oxygen evolution. These electrocatalysts have applications in the efficient separation of oxygen from air for oxy-combustion applications and in the efficient production of hydrogen from water using electrolysis.

Understanding how molecules interact with each other on catalyst surfaces and being able to predict their behavior accurately as a function of concentration is a major challenge. Prof. Kitchin performs quantum mechanical calculations to parameterize simpler, faster models that can then be used to predict and understand the interactions of molecules with metal surfaces.

**Recognition**

Department of Energy Early Career Award
Alexander von Humboldt Postdoctoral Research Fellow, 2004-2005
American Vacuum Society Russell & Sigurd Varian Award, 2003

**Publications**


Evaporation-induced self assembly of infiltrated metal oxide electrocatalysts for applications in water electrolysis, gas separations and solid oxide fuel cells.
Professor Miller’s research interests include characterization of surfaces and surface processes for fundamental understanding of catalysts, separation devices and chemical sensors.

Tools and Methodologies for High-Throughput Materials and Surface Science

The dependence of alloy properties on composition cannot be completely understood based on studies of a few single-composition samples. To address this challenge, Prof. Miller, in collaboration with NETL and Prof. Andrew Gellman, is developing accelerated, or high-throughput, methods for materials and surface science. The CMU-NETL team has developed a set of unique tools for preparation of Composition Spread Alloy Films (CSAFs), samples which contain all possible compositions of a multi-component alloy on a single, compact (~1 cm²) substrate (figure). Current research is focused on preparation of PdCu and PdCuAu CSAFs as model hydrogen separation membrane surfaces, and spatially-resolved characterization of their compositions and catalytic activities. The CSAF platform will enable understanding of the influence of composition on materials performance in a wide variety of applications, including catalysis, corrosion control and lubrication—in a fraction of the time that would be required by a series of traditional, one-composition-at-a-time measurements.

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Recognition

Member of Sigma Xi Scientific Research Society
American Institute of Chemical Engineers
2010 Shining Star Volunteer of the Year Award

Publications


Eranda Nikolla
ASSISTANT PROFESSOR OF CHEMICAL ENGINEERING

Recognition
University of Michigan ProQuest 2009 Distinguished Dissertation Award
Young Scientist Award, International Congress on Catalysis, 2008
Walter J. Weber Jr. Award in Environmental and Energy Sustainability, University of Michigan, 2007

Publications

Prof. Nikolla’s research interests are interdisciplinary and encompass the fields of catalysis, electrocatalysis, computational chemistry, material synthesis and reaction engineering. She uses a combined experimental/theoretical approach aimed at understanding the chemical transformations that occur on catalytic surfaces in order to develop new or improved catalytic and electrocatalytic materials. Future projects will focus in studying various issues related to electrochemical systems (i.e. fuel cells, electrolyzers, batteries) and cooperative/selective catalysis (functionalized heterogeneous catalysts).

Prof. Nikolla has developed robust electrocatalysts for solid oxide fuel cell anodes. She has also investigated biomass conversion to fuels and other chemicals. More specifically she is working on designing robust heterogeneous catalysts for conversion of carbohydrates to valuable chemicals.

Electrochemical systems provide an efficient and clean approach to energy conversion and storage if properties such as material stability and electrochemical activity can be improved. Prof. Nikolla will use controlled synthesis, electron microscopy, spectroscopy, electrochemical measurements and quantum chemical calculations to address these issues and explore cooperative/selective catalysis. State of the art synthesis techniques will be used to make active and robust catalytic materials.

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**a.** Schematic representation of a fuel cell operating with biofuels. The anode of the fuel cell is exposed to the biofuel while the cathode is exposed to air. **b.** Scanning electron micrograph of a solid oxide fuel cell synthesized in the lab.
Professor Pandis’s research areas include the study of multiphase atmospheric chemistry as it relates to photochemical smog and acid deposition, as well as topics related to global climate change.

Control strategies for atmospheric ozone, particulate matter and acidity air pollution problems have been traditionally treated separately from each other, often resulting in suboptimal choices of emission control strategies. The air pollution group is developing comprehensive mathematical models describing the interplay of pollutant emissions, atmospheric homogeneous and heterogeneous chemistry, dispersion and removal processes leading to major air pollution problems. After evaluation against observations, these tools are used for the identification of cost-effective emission controls for the reduction of damages caused by multiple pollutants.

Atmospheric Chemistry and Global Climate Change
The interactions between the anthropogenic perturbations of the atmospheric chemical composition and climate are investigated in a number of projects. These include studies of the role of atmospheric aerosols in the earth’s radiative balance, changes in the oxidative capacity of the atmosphere, the anthropogenic perturbations in the remote marine atmosphere and the long range transport of atmospheric trace components.

Properties of Atmospheric Aerosols
The partitioning of semivolatile atmospheric aerosol components between the gas and particulate phases is investigated. The role of the organic aerosol components in the ability of atmospheric particles to absorb water is a major focus of this research.

Air Quality and Climate Change
The interactions between climate and anthropogenic perturbations of atmospheric chemical composition are investigated in a number of projects. These include studies of the role of atmospheric aerosols in the earth’s radiative balance, changes in the oxidative capacity of the atmosphere, the anthropogenic perturbations in the remote marine atmosphere and the long range transport of atmospheric trace components. We are developing a comprehensive modeling system that can describe air quality and climate at the global scale, but also at the regional and urban scales. This system is used to address questions about the changes in air quality and the emission control strategies that can both improve local air quality and help reduce climate change.

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Professor Prieve’s research interests focus on electrokinetic phenomena and the nature and measurement of colloidal forces.

**Total Internal Reflection Microscopy.** Professor Prieve developed a new experimental technique called Total Internal Reflection Microscopy which can monitor (with nanometer resolution) the elevation of a single microscopic sphere immersed in an aqueous solution and levitated above a transparent plate as the sphere undergoes Brownian motion and interacts with the plate.

**Improved Conversion Efficiency for Dye-Sensitized Solar Cells.** Nanoparticles of TiO$_2$ coated with dye are deposited in a compact layer sandwiched between two planar electrodes. Profs. Prieve and Ydstie hope to improve the efficiency by applying the principles of 2-D electro-assembly to produce more dense layers of particles in more intimate contact with each other and the electrodes.

**New Formulations of Drilling Muds for Very Deep Oil Wells.** Mixtures of clay, barite and a surfactant stabilizer are suspended in either oil or water. Drilling of very deep wells involves extreme conditions of temperature and pressure which can decompose polymeric stabilizers used for shallower wells. Profs. Prieve and Walker propose to use inorganic nanoparticles in place of polymeric surfactants and are exploring the application of “nanoparticle haloing” as the mechanism of stabilization.
Professor Przybycien’s group focuses on research questions in the areas of applied biophysics, drug delivery and biosensor development.

**Applied biophysics** Prof. Przybycien addresses the practical problems and fundamental phenomena associated with the processing and use of pharmaceutical proteins generated by the biotechnology industry. Protein denaturation, aggregation and adsorption phenomena are probed on the molecular level with spectroscopic, optical and biophysical tools. Current topics include overcoming interfacial denaturation in the delivery of proteins from poly(lactide-co-glycolide) microspheres, the impact of micro-scale and nano-scale surface features and curvature on protein adsorption behavior, and more process oriented topics including the use of PEGylation technology to enhance affinity chromatography performance.

**Drug delivery.** Here the emphasis is on using molecular-level insights to improve drug-based therapies. Current topics include enhancing spreading, and mucolysis and antimicrobial activity in pulmonary drug delivery with surfactants.

**Biosensors.** Microelectromechanical systems-based and macroscopic sensors. Current topics include development of a MEMS membrane-based gravimetric sensor for biosecurity, analytical and diagnostic use and development of a hand-held tissue reflectance spectrometer for detection of incipient pressure ulcers regardless of skin pigmentation.

A lumped model for recombinant human growth hormone (rhGH) aggregation. Native and unfolded monomer and dimer fractions of rhGH are connected by unfolding and self-association equilibria which can be measured via biophysical and colloidal tools. The kinetic flux of rhGH into aggregate states will be proportional to the concentration of unfolded dimer species $U_2$.
Professor Sahinidis’s research interests are at the interface between computer science and operations research, with applications in a variety of engineering and scientific systems.

**Informatics Problems in Chemistry, Biology and Medicine.** With the recent accumulation of vast amounts of chemical, biological and clinical data, many scientific fields are becoming increasingly data-driven as opposed to model-driven. This paradigm shift has brought about many challenging computational problems. Even though these problems originate from very disparate fields, they have very similar mathematical structures. In particular, they involve the use of a merit function to evaluate alternatives from very large, typically combinatorial, search spaces. Prof. Sahinidis’s work in this area provides comprehensive and rigorous solutions to inverse imaging problems in X-ray crystallography, modeling and estimation of dynamic metabolic and signaling pathways, structural bioinformatics, medical diagnosis and prognosis, and the design of novel chemicals that are environmentally benign. In all cases, models from first principles are developed to guide the extraction of information from experimental data.

**Optimization Theory, Algorithms and Software.** A plethora of problems in science and engineering require the solution of nonlinear optimization problems with multiple local solutions. Since the early 1990s, Prof. Sahinidis’s research pioneered the development of an all-purpose, rigorous global optimization methodology. His results have included powerful domain reduction strategies, sharp relaxations for nonconvex optimization problems, an entirely linear outer-approximation scheme for global optimization, finite branching schemes for certain continuous optimization problems, and the global optimization software BARON. Scientists and engineers have used BARON in many application areas, including the development of new Runge-Kutta methods for partial differential equations, energy policy making, modeling and design of metabolic processes, product and process design, engineering design and automatic control. The ultimate goal of this research is to provide precise and valuable computational optimization tools that will make possible the solution of problems that are currently considered intractable. Towards this end, current projects pursue fundamental advances in linear optimization and optimization without algebraic models. While general in purpose, the algorithms are developed and validated through several applications, including critical problems in energy process modeling and optimization.
Professor Schneider’s work focuses on the development of novel colloidal and biomolecular materials for bioanalytical devices, pharmaceutical processing and drug delivery.

**Rapid, Gel-Free DNA Electrophoresis using Surfactant Systems.** The use of gels and other polymer systems to electrophoretically separate DNA limits separation speed due to the high friction encountered. Length-based resolution can be realized in a gel-free matrix using dilute, low-viscosity surfactant solutions. Above their CMC, nonionic surfactant micelles bind to chemically modified ends of the DNA to provide drag. Additionally, micelles undergo rapid, spontaneous fluctuations in size when attached to DNA during electrophoresis. These fluctuations ensure that each DNA in the population experiences a nearly identical drag as required for high resolution. Current efforts center on developing microfluidic devices that best leverage this rapid electrophoresis platform.

**DNA and RNA Purification using Peptide Nucleic Acid Amphiphiles.** Peptide nucleic acids (PNAs) are synthetic materials that hybridize with complementary DNA and RNA with great sequence selectivity. Prof. Schneider’s group has developed a series of PNA amphiphiles that self-assemble in solution and bind tightly to nonpolar chromatographic media while retaining their unique DNA binding properties. These materials are ideal for affinity-based separations of DNA and RNA as hybridization occurs in solution, free of biasing surface effects. Current efforts focus on ultrasensitive isolation of microRNAs from biological samples, with applications in early detection of cancer.

**Wetting Dynamics using Atomic Force Microscopy (AFM).** The dynamics of film formation play a critical role in the behavior of disk-drive lubricants and biofilms. Prof. Schneider’s group uses the AFM to interrogate the formation and breakage of liquid bridges formed between AFM probes and chemically modified surfaces over millisecond time scales. In some cases, sub-monolayer flow processes dictate the speed of bridge formation, and these flows can be controlled by appropriate surface chemistry. Current work involves incorporating surfactants into thin films to study effects of Marangoni stresses on these processes.
Professor Sides investigates topics in electrochemistry, electrochemical engineering and colloid science. He studies forces that move microparticles laterally on electrodes when electric fields are applied normally to the electrolyte/electrode interface. While most investigators have concentrated on observing the in-plane motion, Prof. Sides and Prof. Prieve have been using Total Internal Reflection Microscopy in combination with a fully equipped electrochemical cell to measure the out-of-plane motion, seeking clues to complex direct and induced forces that move the particles. This work has led to invention of a technique for high-throughput testing of electrocatalytic alloys, as shown in the figure.

Professor Sides has also invented a novel instrument based on a rotating disk for quick and convenient determination of the zeta potential of macroscopic (> 1 mm significant dimension) surfaces. The zeta potential of a surface is a characteristic of its electrostatic state; for particles, zeta potential helps determine the stability of dispersions. Prof. Sides and his students are using it to observe deposition of nanoparticles in real time. This technology also is currently being applied to the characterization of polishing pads and brushes for planarization of wafers during fabrication of integrated circuits.
Research in Professor Tilton’s group emphasizes the use of interfacial physical chemistry to engineer complex fluid and particulate systems.

**Emulsifiers Based on Nanoparticle-Grafted Polymer Brushes.** Liquid-liquid dispersions, or emulsions, find diverse applications in pharmaceuticals, cleaner-burning diesel fuels, personal care products, polymer manufacturing and other technologies. Pickering emulsions are a special case where dispersed liquid droplets are stabilized by adsorbing colloidal particles, rather than molecular surfactants, at the liquid/liquid interface. This group is developing inorganic core/polymer brush shell nanoparticles as high efficiency Pickering emulsifiers. At concentrations as low as a few hundredths of a weight percent, these nanoparticles produce emulsions with extremely long shelf-lives.

**Environmental Impacts of Engineered Nanoparticles.** Commercial usage of materials that incorporate engineered, often highly reactive, nanoparticles is increasing at a rapid pace, and commonplace routes exist for such nanoparticles to accumulate in the environment. Though much uncertainty exists, a growing body of research indicates the potential for certain engineered nanoparticles to detrimentally affect microbes, plants and animals in the environment. This group focuses on how natural organic macromolecules, that inevitably coat all engineered nanoparticles once they enter the environment, subsequently control their microbial interactions. The key question is whether these coatings have sensitizing, passivating or insignificant effects on nanoparticle interactions with microbes.

**Self-Dispersing Surfactant Drug Carriers for Pulmonary Drug Delivery.** Patients with obstructive lung disease, such as cystic fibrosis, often suffer from persistent bacterial infections of the lung. Inhaled aerosol delivery of antibiotics is desirable to treat lung infections, but obstructed airflows often prevent aerosolized antibiotics from reaching infections. This group is developing aerosolized surfactant formulations that maximize drug spreading over large areas of the airway surface and promote antibiotic diffusion to mucus-sheltered infections. This work is performed in collaboration with the Garoff and Przybycien groups at Carnegie Mellon and pulmonary medicine researchers at the University of Pittsburgh School of Medicine.
The objective of Professor Walker’s research is to quantify the relationship between molecular-level interactions and macroscopic fluid behavior. Her group has developed experimental tools and techniques for systematically controlling molecular-level behavior, characterizing nanoscale and microscale structure in fluid systems and quantifying rheology and flow behavior of complex fluids.

Part of the research focuses on design and control of nanoscale structure in complex fluid systems. Using a combination of synthesis and manipulation of colloidal interactions, her group is developing novel soft materials such as elongated, or wormlike, micelles based on ionic surfactants. Variation of counterions allows control of the rheology and phase behavior of these materials for a variety of applications. Further adaptation of counterion chemistry makes the use of these nanoscale structures as templates for generation of amphiphilic rod-like nanoparticles possible. Another example is recent work on using the structure inherent in block copolymers to develop spatially-structured nanocomposites. Understanding the formation of these nanocomposites allows development of applications in separation, delivery and protein stabilization.

A second research focus is the impact of viscoelasticity on deformable interfaces under flow. Many industrial processes including ink jet printing, spraying and blending involve deformable liquid-vapor or liquid-liquid interfaces. In all of these processes, colloidal and polymeric fluid additives add elasticity to fluids and, hence, add a second elastic behavior with very different timescales than those inherent to the interfacial process. Prof. Walker’s group investigates the role of fluid elasticity on these complex processes. Current work focuses on a fundamental study of how polymeric solutions wet solid surfaces and on an applications-based study of how protein additives alter ink jet printing in the formation of three-dimensional biomimetic materials.

A collaboration with Shelley Anna has two students developing approaches to the use of two phase flow in microfluidic devices for chemical processing. The projects require detailed understanding of fluid mechanical phenomena so that the behavior can be harnessed to produce “nanoreactors” that have sized driven by, but decoupled from, the device sizes. Recent findings demonstrate our ability to generate submicron droplets in these reactor systems and control the size distribution of gold and platinum nanoparticles grown in microreactors.
B. Erik Ydstie
PROFESSOR OF CHEMICAL ENGINEERING, PROFESSOR OF ELECTRICAL ENGINEERING AT CARNEGIE MELLON (COURTESY), PROFESSOR II OF ELECTRICAL ENGINEERING AT NUST, TRONDHEIM, NORWAY

Professor Ydstie’s group develops methods for stable and robust control and optimization of chemical processes that combine physical models and online learning.

Design and control of particulate processes with application to Solar Cell production. Prof. Ydstie develops models and control strategies for solar grade silicon production. Solar grade silicon is in high demand due to the very rapidly growing interest in using solar cells to generate electricity for domestic uses, telecommunications and distributed power generation in the third world. This investigation is aimed towards design and control of fluidized bed reactors for decomposition of silane.

Dynamics and Control of Complex Process Networks. Prof. Ydstie introduced a framework for studying dynamics, distributed control, and optimization of complex networks. These networks represent self-organizing structures so that stability and optimality follow as a consequence of how the networks are put together and how they are connected with other networks. The class is sufficiently broad to cover process networks, biochemical networks, reaction networks, and supply chains. The study has led to a decomposition of the business decision making processes, optimal behaviors and decentralized decision making. The formalism of irreversible thermodynamics and the passivity theory of nonlinear control is a basis for this theory.

Real Time Adaptive Control and Optimization. Online optimization techniques for constrained and unconstrained optimization using input/output data are being developed. The aim is to make stand-alone optimization modules that gather information by simulation and/or experimentation and adaptively control the process so that over time the optimizer converges to the optimal decision maker. The optimizer is based on a method referred to as Q learning which was developed in the area of computer science for optimal control of discrete and continuous Markov decision problems. Prof. Ydstie’s group adapted the method for real time process control and developed a theoretical foundation for online decision making using adaptive control theory. The advantages of the adaptive methods over other traditional optimization approaches are that it uses current process models to develop policies and that they are self-learning in the sense that they adapt as process conditions change.

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Recognition
CAST award of the AIChE, 2007
13th RWH Sargent Lecture Imperial College, London, 2006
Distinguished Lecturer, University of Alberta, 2005
Automatica, Associate Editor, 1993-1999

Publications


FREQUENT ANSWERS

Graduate Degrees 33
Graduate Student Life 34
Graduate Student Profiles 34
Facilities 37
Research Centers 39
Awards and Funding 41
The Department of Chemical Engineering at Carnegie Mellon University grants the doctoral degree and four master’s level degrees. Ph.D. students are fully supported by fellowships or by the department; however, master’s students must have independent sources of financial support.

Ph.D. Program

The Ph.D. degree, the highest level, provides the deepest foundation in coursework and the experience of completing a major research project leading to a dissertation. The typical student enters with a B.S. in chemical engineering and emerges 4.7 years later with the Ph.D. degree. Students must take 4 core chemical engineering courses (out of a menu of 6), a graduate chemical engineering course and 3 – 5 other courses. The distribution is usually 6 or 7 courses in chemical engineering and 1 or 2 courses in other fields. Students must complete teaching assistant assignments, but this commitment is usually restricted to about 5 hours per week over three semesters. Students begin their research during the first year of residence and take the oral research-based Qualifying Exam at the end of the first year. Approximately a year after taking the Qualifying Exam, Ph.D. students must pass a Ph.D. proposal in which the student presents the main themes and methods of their proposed thesis to his/her committee.

Students entering the Ph.D. program with an M.S. degree in chemical engineering from another university must take 4 – 6 courses and usually complete the degree in about 4 years.

Research advisor selection considers student preferences, faculty availability and project funding. During the first semester in residence, a new graduate student meets each faculty member to discuss research projects under way or planned. After interviewing all prospective advisors, the student indicates three choices for a thesis advisor, in order of preference. The department head makes the assignments of advisors based on this student input and input from the faculty.

M.S. Program

Students entering the M.S. program acquire both advanced education in engineering science and design, and they complete an original research project under the supervision of a research advisor. Students entering the M.S. program take 4 out of a possible 6 core chemical engineering courses and 2 – 4 other courses. The M.S. student also must write a thesis based on their research. The typical time to completion is 16 – 21 months.

M.Ch.E. Program

The M.Ch.E. program is designed to raise the student’s level of coursework knowledge to the graduate level of understanding in core chemical engineering and to provide flexibility for the student to take other courses helpful for their career. The MChE student takes 4 out of a possible 6 core graduate courses, an advanced chemical engineering graduate course, and 3 – 4 other courses of his/her choosing. For example, the student can emphasize chemical engineering, other engineering, business education, or math and other sciences.

The time to completion, assuming entrance with a B.S. in chemical engineering, is two semesters if a normal course load is taken. Students have begun and completed this degree starting from other scientific disciplines such as chemistry, but the time required is often one or two additional semesters.

M.S. in Energy Science, Technology and Policy:

The College of Engineering offers a Master’s in Energy Science, Technology and Policy program intended for students who seek a Master’s program that emphasizes both engineering and a broader perspective in economics and public policy. Students enroll in the program independent of a department but can select a disciplinary concentration within chemical engineering. Requiring 8 – 10 courses to complete, the degree is designed to be finished in one academic year. Students in this program acquire a unique education focused on energy and incorporating strengths from other engineering departments.
Secondary Organic Particulate Matter: Measurements, Models and Mitigation

Lea Hildebrandt

Lea received her B.S. degree in Chemical Engineering from Caltech and is a 4th year doctoral student in the Environmental Engineering Group.

Submicron atmospheric particles have a highly uncertain effect on climate, and they adversely affect human health. Organic aerosol globally comprises a significant fraction (20 – 90%) of the submicron particle mass but it is not well understood. The goal of Lea’s research is to improve our understanding of the processes governing the properties and concentrations of organic aerosol in the atmosphere through a series of laboratory experiments and ambient measurements. She implements the findings from these studies in a three-dimensional chemical transport model and then tests the model against observations. The improved model can be used to evaluate different emission control options for reducing organic aerosol concentrations and their adverse effects.

Her laboratory experiments and ambient measurements focus on investigating the initial formation, mixing and aging of organic aerosol. Most chemical transport models assume that organic aerosol components from different sources form a single solution. This is a critical assumption which greatly affects modeled organic aerosol concentrations, but the assumption has not been confirmed experimentally. Lea conducted novel experiments using a High Resolution Time-of-Flight Aerosol Mass Spectrometer and isotopically labeled compounds to confirm that anthropogenic and biogenic secondary organic aerosol components form a single solution.

L. Hildebrandt, N.M. Donahue, S.N. Pandis, Atmospheric Chemistry and Physics, 2973 (2009).
L. Hildebrandt et al., Atmospheric Chemistry and Physics 10, 4167 (2010).

Graduate Student Life

Graduate students in ChemE at CMU immediately become members of a club. ChEGSA is the student organization for all graduate students in the Department of Chemical Engineering, and it serves as the liaison between the graduate students and the faculty, staff and undergraduate students. All chemical engineering graduate students automatically become members of ChEGSA upon matriculation to the department. You can participate as much or as little as you like; ChEGSA is a community available to you from your first day on campus.
An Experimental and Theoretical Study of Surfactant Dynamics at Microscale Interfaces

Nick Alvarez

Nick Alvarez graduated from the University of Florida with a Bachelor’s Degree in Chemical Engineering and entered the doctoral program at CMU as a National Science Foundation Graduate Fellow.

Nick works in the Complex Fluids Engineering group on transport phenomena and the dynamics of amphiphilic molecules at highly curved interfaces. A scaling analysis has shown that the rate of adsorption by diffusion depends on interface curvature. The higher the radii of curvature, the faster the molecules are transported to the interface via diffusion. This scaling has been confirmed both numerically and experimentally. Nick designed a new microtensiometer apparatus to measure the adsorption of amphiphilic species to microscale bubbles; this requires less volume and allows faster measurement compared with other dynamic surface tension techniques. Nick has a passion for teaching and mentoring students, for which he was awarded the Mark Dennis Karl Graduate Teaching Award in Spring 2010. In addition, he received the ChEGSA Symposium Award in 2009. Nick is looking forward to a career in academia.


One of the most vibrant and unique organizations of its type, ChEGSA sponsors a number of events throughout the year, both social and professional. The most frequent social activity is the weekly happy hour, held every Friday afternoon in the graduate student lounge on the A-level of Doherty Hall. The happy hours provide a relaxed atmosphere for interaction among faculty, staff and graduate students or just some ping pong with friends. In addition to the happy hours, ChEGSA hosts a number of social gatherings throughout the year. A welcome party for the new graduate students and a holiday party in December are annual traditions. Other department outings have included Super Bowl parties, hiking/camping at Cooper’s Rock, a wine and cheese event, skiing at Seven Springs, tailgating at a Pirates’ game, an international potluck dinner and a spring luau. ChEGSA also organizes intramural teams in a variety of sports.

On the professional side, the most significant ChEGSA event held annually is the Graduate Student Research Symposium. Over 30 years ago, ChemE
at CMU was the first to conduct an intradepartmental symposium completely run by graduate students. Senior students present their research to the entire department over a two-day event, promoting communication within the department and giving new graduate students an early introduction to the ongoing research thrusts during their process of identifying a research advisor. Also, prizes are awarded for the best talks. Industrial sponsors send financial support and representatives to the event annually.

In summary, ChEGSA provides immediate connection to students at all stages of their degrees as well as to your entering classmates. It is a vital organization in the department.
Facilities

Doherty Hall

The Department of Chemical Engineering at Carnegie Mellon occupies Doherty Hall located at the center of the campus. Originally constructed in 1908 and expanded significantly in the 1950s, Doherty Hall underwent a massive $27M renovation completed in the Fall of 2008. This renovation created modern new experimental laboratories, computational facilities and office space for students, researchers and faculty. The department occupies about 26,000 square feet of experimental laboratory space and about 18,000 square feet of office space and computational labs in addition to the space allocated to faculty offices, department offices and teaching laboratories. The department has adopted a modern philosophy in its laboratories which have an open architecture allowing several different research groups to share space.

Each of four floors of the main laboratory wing are large, open research labs of about 3,500–4,000 square feet each. Each floor is home to a group: Complex Fluids Engineering, Bioengineering, Catalysis and Surface Science, and Envirochemical Engineering. The fourth floor space is a new office complex for the Process Systems Engineering group. The shared nature of these labs and offices allows much easier reassignment and modification of laboratory space as research projects ebb and flow. Furthermore, this architecture reflects and fosters a collaborative and interdisciplinary culture for the students working in this environment.

The renovation of Doherty Hall was a very exciting development for Chemical Engineering. Each of the focused research groups maintains a support facility. The CPS Lab supports the Complex Fluids group. The Beowulf cluster supports the Process Systems group. These facilities are briefly described here.

PPG Industries Colloids, Polymers and Surfaces (CPS) Laboratory

The PPG Industries Colloids, Polymers and Surfaces Laboratory, a unique 2,200 square foot facility supporting the complex fluids research group, is used both for instruction and research. The CPS lab provides the capability for characterization of fine particles, macromolecules, interfaces and the complex fluids formed by combinations of these materials. Lab courses in colloid and polymer characterization are offered at both the undergraduate and graduate levels. The hands-on laboratory experience features 27 experiments and demonstrations. Offering laboratory courses every semester to 25 – 30 students, CPS lab personnel train about 40 students per year including undergraduate, masters and doctoral students working on independent research projects in most of the engineering and science departments at Carnegie Mellon.

Physical property measurement capabilities in the lab include surface and interfacial tension, particle sizing, contact angle, rheology, static and dynamic light scattering, membrane osmometry, differential scanning calorimetry, UV-VIS spectrophotometry, mechanical property testing, conductivity, critical micelle concentration measurements, powder surface area, electrophoretic mobility of colloids and dynamic surface tension. The laboratory is also used for outreach events that provide hands-on science experiences for K-12 students and teachers to promote science and engineering.

Beowulf Cluster

The department operates a high performance computing cluster in a dedicated, cooled, computing room. Funded by the College of Engineering and ChemE, the cluster consists of rack-mounted computing nodes connected by a gigabit and infiniband network. The cluster contains 20 nodes with a total of 640 AMD computing cores with 2 TB of RAM distributed across the nodes. A 2 TB file server provides disk space for users to set up their own computing environment. The cluster is operational year round.

The main uses of the cluster include computational chemistry (Professor Kitchin) and large-scale optimization (Professor Biegler) as well as molecular
simulations by groups outside the department. Individual jobs run anywhere from a few hours to several weeks and can use multiple processors if needed. All jobs are continuously tracked through a web based monitoring system and the allocation of computing resources is managed by a queue system to ensure efficient throughput in a user friendly manner. Sharing the cluster between multiple research groups with different usage patterns provides a flexible computational environment in which each student or postdoc can run a large number of simultaneous jobs when needed.

Surfaces Lab

ChemE houses a fully functional surface analysis laboratory that supports the Catalysis and Surface Science group. The laboratory has eight versatile ultra-high vacuum, surface preparation and analysis chambers equipped with state-of-the-art instrumentation. Many of these chambers and ancillary equipment were constructed at Carnegie Mellon; some of the capabilities are unique. The instrumentation in the laboratory includes: five X-ray photoemission spectrometers, two ultra-violet photoemission spectrometers, an Auger electron spectrometer, six low energy electron diffraction optics, two high resolution electron energy loss spectrometers, a variety of mass spectrometers, two Fourier transform infrared spectrometers, low energy ion scattering spectrometer and an ultra-high vacuum tribometer. The microscopy instrumentation includes a secondary electron microscope a scanning Auger microscope and an electrochemical scanning tunneling microscope. In addition, the laboratory has instrumentation for surface preparation by magnetron sputter deposition, thin film evaporation and molecular deposition. The Catalysis and Surface Science group has access to a variety of instrumentation located at the National Energy Technology Lab.

The Air Quality Lab

The Air Quality Laboratory is newly renovated for the Center for Atmospheric Particle Studies with state-of-the-art facilities and equipment. Work modes include both laboratory-scale studies of atmospheric chemistry as well as field campaigns. The equipment can be easily moved from one experiment to another as needs dictate. The facilities in the Air Quality Laboratory include: a 16 cubic meter temperature-controlled smog chamber, two clean rooms, a mobile laboratory for field measurements, an aerosol flow reactor and a high-pressure discharge flow reactor. In addition, the laboratory houses several major pieces of instrumentation including: an aerosol mass spectrometer, a proton transfer reaction mass spectrometer, several scanning mobility particle size spectrometers, a cloud condensation nucleus counter, a thermal denuder for particle volatility measurement, two Fourier transform infrared spectrometers, a UV-VIS spectrometer and several gas chromatograph-mass spectrometers.

Mammalian Cell Culture and Bioimaging

Facilities for microbial cell culture include 1- and 5-liter batch fermentors with monitoring and control of pH and dissolved oxygen and mass-spectroscopy monitoring of fermentation off-gas. Also, molecular biology facilities are linked with the microbial biotechnology facilities. Two PCR thermocyclers are available, including a 16-cuvette system with realtime fluorescence monitoring for quantitative PCR. For high throughput production of recombinant DNA and recombinant protein a 10 liter incubator shaker, a 6 liter capacity centrifuge and an Äkta protein purification system housed in a separated 4°C cold room are available. Large-scale, automated autoclave and glass washing equipment is located in adjacent rooms, along with several -80°C bench freezers, ultra-centrifuge systems, a Speed-Vac concentrator and lyophilizer. Characterization of recombinant molecules is available with three UV-VIS spectrophotometers, circular dichroism, fluorimetry and other equipment in the Biointerfaces Laboratory. A centralized electrophoresis facility includes equipment for agarose gel and polyacrylamide gel electrophoresis and Western blotting.

Mammalian cell culture and live cell imaging are available in BSL-2 designated facilities. Two laminar-flow, biosafety hoods are available for tissue culture; one is designated for rDNA manipulation of cells and one for research of cells with artificial materials. Characterization of cells is available with a tabletop flow cytometer, a Coulter counter and three inverted epifluorescence microscopes. The live cell imaging facility includes a fully automated microscope enclosed in an environmental chamber (temperature and CO₂). Microscopy capabilities include brightfield, phase, polarization, fluorescence imaging, time lapse and deconvolution. Biophysical cellular characterization attachments include parallel plate flow chambers, micropipette aspiration, TIRF (total internal reflection fluorescence), FRAP (fluorescence recovery after photobleaching) and microinjection.

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Research Centers

Center for Advanced Process Decision-making (CAPD)

FACULTY: BIEGLER, GROSSMANN, YDSTIE, SAHINIDIS  HTTP://CAPD.CHE.ME.CMU.EDU

The CAPD provides an umbrella organization for interactions with industry in the Process Systems Engineering area. Based on fundamental research in modeling, optimization and control, the CAPD addresses product and process design (i.e., design of molecules, solar and fuel cells, biomass processes, metabolic networks, separation networks and energy systems), process control and safety (i.e., adaptive control, passivity theory, fault trees, nonlinear control), enterprise-wide optimization (i.e., scheduling, planning and control of supply chains) and systems biology (i.e., metabolic networks and biomolecular design). These applications are addressed through methodologies based on process modeling (i.e., dynamics, superstructures), mathematical programming (i.e., nonlinear and mixed-integer programming, global optimization, stochastic programming), modern search methods (i.e., logic-based and hybrid methods), and advanced computing (i.e., Beowulf cluster).

Current members of CAPD include: ABB, Air Products, Bayer, BP, Cognizant, Collaboratory for Process & Dynamic Systems Research, Dash Optim., Dow, Eastman, Ecopetrol, ExxonMobil, GAMS, Kraft, NOVA Chemicals, Neste Eng., Paragon Decision Tech., Petrobras, Pfizer, PPG, Praxair, Total and Unilever. These companies support CAPD research through membership fees and special industrial projects. There are also special interest groups within CAPD:
1) Enterprise-wide Optimization, where the goal is to develop a comprehensive set of computational capabilities for addressing the integrated planning, scheduling, real-time optimization and inventory control of process systems; and
2) Energy Systems Initiative, in which companies provide case studies that are undertaken by students and researchers of the CAPD.

Students are involved in the CAPD through an annual review meeting where they present their work and meet industrial researchers. In addition, graduate students can obtain summer industrial internships through the CAPD.

Center for Complex Fluids Engineering (CCFE)

FACULTY: ANNA, DAHL, PRIEVE, PRZYBYCIEEN, SCHNEIDER, SIDES, TILON, WALKER, PLUS FACULTY FROM SCIENCE AND OTHER ENGINEERING DEPARTMENTS. HTTP://CFE.CHE.ME.CMU.EDU/

The Center for Complex Fluids Engineering is an interdisciplinary research and educational effort serving two different colleges at Carnegie Mellon University. Faculty and graduate students of the Complex Fluids Engineering group participate in the center; they perform fundamental and applied research to attack problems in the formulation, control and engineering of processes and materials involving complex fluids. Complex fluids, which include polymeric and surfactant solutions as well as colloidal suspensions, are of universal industrial importance due to their unique mechanical properties, their capacity to solubilize and transport materials and their internal microstructures. The CCFE is a synergy
of scientific knowledge bases targeted at processing operations involving complex fluids in the coatings, pharmaceutical and mining industries such as spraying, granulation, solid/liquid and protein separations. This same scientific knowledge base is vital to the fields of nanotechnology, environmental engineering, and biotechnology, areas of significant research by CCFE faculty.

Center for Atmospheric Particle Studies (CAPS)

FACULTY: DONAHUE AND PANDIS PLUS FACULTY FROM CIVIL AND ENVIRONMENTAL ENGINEERING AND MECHANICAL ENGINEERING
HTTP://CAPS.WEB.CMU.EDU/

The Center for Atmospheric Particle Studies addresses the effect of fine particulate matter on the environment, human health and global climate. Fine particulate matter consists of particles with diameters less than 2.5 micrometers (PM2.5). These particles have significant adverse health effects but also play a crucial role in the climate cycle, both by directly scattering light and by seeding cloud droplets. The goal of CAPS is to integrate interdisciplinary research over the full range of scientific and engineering questions surrounding fine particulate matter and to integrate findings into policy-relevant analyses through collaboration with the department of Engineering and Public Policy (EPP). Faculty members in CAPS are world leaders in research and policy associated with ambient PM. Most research projects are collaborations including several CAPS members. Roughly 25 doctoral students are active in CAPS, working on research projects including computer modeling work, laboratory experimentation and in-situ observation. A large portion of the laboratory research is conducted in the Air Quality Laboratory (see p. 38) and field work is enhanced by an instrumented mobile laboratory.

National Energy Technology Laboratory – Regional University Alliance

FACULTY: BIEGLER, GELLMAN, GROSSMANN, KITCHIN, MILLER, SAHINIDIS, WALKER, YOSTIE
WWW.CHEME.CMU.EDU/RESEARCH/CENTERS.HTM

The Department of Chemical Engineering at Carnegie Mellon has spearheaded the formation of a collaborative energy research institute including faculty from a variety of departments across Carnegie Mellon, four outside universities and the Department of Energy – National Energy Technology Laboratory (NETL). Professor Gellman leads the effort of the NETL – Regional University Alliance (RUA) at Carnegie Mellon.

The goal of its energy research portfolio is to address the problems associated with the socially and environmentally responsible use of existing energy sources and the development of alternative sources for the future. The NETL-RUA research portfolio is funded at a level of ~$20 M/yr. The research portfolio covers the full range of problems related to fossil fuel energy use and is aligned with the research focus areas of the NETL:

1. Computational and basic science
2. Energy system dynamics
3. Geological and environmental systems
4. Materials science and engineering
AWARDS AND HONORS 2000 – 2010

2010
Nick Sahinidis—AIChe CAST Computing in ChemE Award
Krish Dahl—NSF CAREER Award
John Kitchin—DOE Early Career Award
Jim Miller—AIChe Service Award
Robert Tilton—Fellow of the American Chemical Society
Todd Przybycien—Fellow of AIChe

2009
Robert Tilton—Member, NIH Nanotechnology Study Section
Larry Biegler—ICS Prize of the INFORMS Computing Society
Larry Biegler—"Olaf Hougen Visiting Professor"
Todd Przybycien—Erskine Fellow, New Zealand
Biegler, Westerberg, Grossmann—AIChe Warren K. Lewis Award

2008
Ignacio Grossmann—“Top 100 Chemical Engineers of Century”
Herb Toor—“Top 100 Chemical Engineers of Century”
Mohammad Islam—Kavli Fellowship
John Kitchin—Wimmer Faculty Fellow

2007
Erik Ydstie—AIChe CAST Computing in ChE Award
Larry Biegler—CACHE Award
Mohammad Islam—Alfred P. Sloan Fellow
Mohammad Islam—NSF CAREER Award

2006
Nick Sahinidis—MPS Beale-Orchard-Hays Prize

2005
Shelley Anna—NSF CAREER Award

2004
John Kitchin—Alexander von Humboldt Fellowship
Ignacio Grossmann—AIChe Fellow
Dennis Prieve—AIChe Fellow
Larry Biegler—AIChe Fellow
Nick Sahinidis—INFORMS Computing Society Prize

2003
Ignacio Grossmann—INFORMS Computing Society Prize
Ignacio Grossmann—Fulbright Senior Lectureship

2002
Steinar Hauan—AIChe Ted Peterson Award
Ignacio Grossmann—ISI Top 15 Most Cited Authors in Computer Science
Ignacio Grossmann—Fellow of INFORMS
James Schneider—Beckman Young Investigator Award

2001
Andrew Gellman—Robert A. Welch Foundation Lecturer
John Anderson—Fellow of AAAS
James Schneider—NSF CAREER Award
Lee White—AIChe Thomas Baron Award
Lynn Walker—NSF CAREER Award
Shelley Anna—Achievement Award, Solutia

2000
Larry Biegler—AIChe CAST Computing in ChE Award
Ignacio Grossmann—National Academy of Engineering
Spyros Pandis—AAAR Whitby Award

FUNDING SOURCES

Federal & State:
Defense Advanced Research Projects Agency
Department of Energy
Environmental Protection Agency
Health Resources Services Administration
DOE—National Energy Technology Lab
National Aeronautics and Space Administration
National Institutes of Health
National Science Foundation
Pennsylvania Infrastructure Technology Alliance

Corporate:
ABB
Air Products and Chemicals
Alnylam
Bayer Foundation
Bayer MaterialScience
BP
Bristol-Meyers Squibb
Cognizant
Dow Chemical
Dash Optimization
Eastman Chemical
Ecopetrol
Environ
ExxonMobil
GAMS Development
Intel
Kraft
Lubrizol
Merck
Mine Safety Appliances
Neste Engineering
Nova Chemicals
Paragon Decision Technologies
Petrobras
PPG Industries
Pfizer
Praxair
Procter & Gamble
Respironics
A.P. Sloan Foundation
Solar Grade Silicon LLC
Total
Unilever
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In addition, Carnegie Mellon University does not discriminate in admission, employment or administration of its programs on the basis of religion, creed, ancestry, belief, age, veteran status, sexual orientation or gender identity. Carnegie Mellon does not discriminate in violation of federal, state, or local laws or executive orders. However, in the judgment of the Carnegie Mellon Human Relations Commission, the Presidential Executive Order directing the Department of Defense to follow a policy of, “Don’t ask, don’t tell, don’t pursue,” excludes openly gay, lesbian and bisexual students from receiving ROTC scholarships or serving in the military. Nevertheless, all ROTC classes at Carnegie Mellon University are available to all students.

Inquiries concerning application of these statements should be directed to the Provost, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, telephone 412-268-6684 or the Vice President for Campus Affairs, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, telephone 412-268-2057.

Carnegie Mellon University publishes an annual campus security report describing the university’s security, alcohol and drug, and sexual assault policies and containing statistics about the number and type of crimes committed on the campus during the preceding three years. You can obtain a copy by contacting the Carnegie Mellon Police Department at 412-268-2323. The security report is available through the World Wide Web at www.cmu.edu/police/.


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