

# *Chemical Engineering at . . . The University of Wisconsin*



Bryce Richter, University of Wisconsin-Madison

*The Memorial Union Terrace, on the shores of Lake Mendota, is a popular spot for eating, relaxing, studying, and sailing.*

## **IF YOU WANT TO BE A BADGER...**

Every schoolchild in Wisconsin learns that the state motto is “Forward,” the state animal is the Badger, the state dance is the Polka, and the official state beverage is Milk. As the only chemical engineering department in the state, public or private, the Chemical and Biological Engineering (CBE) Department at the University of Wisconsin (UW) embraces all of these as part of our heritage and culture. The department especially embraces the “Forward” motto in its research and education efforts. We’ll begin by highlighting three research foci.

## **GLBRC: GREEN INTO GOLD**

UW is home to the Great Lakes Bioenergy Research Center (GLBRC), one of three centers in the nation funded by DOE to the tune of \$125 million over five years. GLBRC is a consortium of researchers from UW and Michigan State University, working in collaboration with national labs and industrial partners, to develop a suite of new technologies to convert cellulosic plant biomass to energy sources. CBE faculty involved with GLBRC include **Jim Dumesic, Manos Mavrikakis, Brian Pflieger, Jennie Reed, and Christos Maravelias**. Their work spans all length scales, from molecular engineering to systems and economic analysis.

Jim Dumesic and his research group are pioneers in the conversion of lignocellulosic biomass to fuel and chemical grade compounds by means of heterogeneous catalysis. Jim uses his expertise in microcalorimetric and spectroscopic techniques to develop new catalytic processes for the conversion of biomass feeds to valuable end products. Jim works closely with Manos Mavrikakis, to tap his expertise in catalyst design from quantum mechanical first principles. The main strategy is to first deconstruct lignocellulose through controlled deoxygenation to obtain platform molecules (5-6 carbons) and monofunctional species that retain functionalities. These can then be reconstructed through upgrading reactions, and tailored to specific new purposes. Highlights from recent work include the production of H<sub>2</sub> and alkanes through aqueous-phase reforming of sugars, and conversion of sugars and sugar alcohols over a Pt-Re based bimetallic catalyst to a mixture of mono-functional intermediate molecules, such as alcohols, ketones and carboxylic acids. One of their most recently developed catalytic strategies is for the production of jet fuels starting from biomass through an integrated system for hydrogenation, decarboxylation, and oligomerization reactions.

Where Jim and Manos use synthetic chemistry, Brian Pflieger uses synthetic biology in the search for new biomass conversion pathways. Synthetic biology is the design and construction of new biological components and systems, and the re-design of natural biological systems, for useful purposes. Brian's research group is developing tools for engineering biological systems in order to design biological catalysts for producing high-value products from renewable resources. Fossil fuels are the raw materials for an enormous diversity of products such as plastics, solvents, and organic building blocks. Conventionally, conversion from fossil fuel to products is carried out through synthetic chemistry and processes familiar to any chemical engineer. As fossil fuel supplies decrease, Brian believes that it is time for synthetic biology to step in, as an alternative approach for manufacturing existing materials as well as a route to totally novel compounds. Currently, his group is engineering microorganisms to produce polymer precursors and diesel fuels.

Jennie Reed takes a systems biology approach, utilizing both experimental and computational approaches to study biological networks. Jennie and her team are building, analyzing, and utilizing metabolic and regulatory models of organisms involved in biofuels. These models are used to evaluate the capabilities of different organisms from a network-based perspective and to identify ways in which genetic manipulations could enhance their productivity. She also develops computational methods for designing strains or cell lines with enhanced production yields of desired products. These computational methods account for both metabolic and regulatory effects occurring inside the cell, and can identify metabolic or regulatory roadblocks that limit production in developed strains.

To be economically viable, any biomass-to-fuels strategy must be coupled to efficient conversion of biomass-derived oxygenated compounds to high-value chemicals. Although several pathways for these conversions are known, it is not established which high-value chemicals should be produced to make the overall process economically attractive, and how chemical and biological approaches should be integrated. Christos Maravelias and his research group have developed a network design approach, where existing fossil-fuel-based and emerging biomass-based technologies are considered. They formulate optimization models to evaluate in a systematic manner a large number of alternatives, and thereby address a series of challenging questions: Which chemicals can be produced most efficiently from biomass? Which emerging technologies could have the greatest impact? Can biomass-based technologies be used today to replace fossil-fuels technologies?

These combined efforts of several UW research groups, along with their collaborators on campus and beyond, are sure to move "Forward" the efforts to build a new biomass-based chemical and fuels economy, while protecting and preserving our natural resources.

## WID: GOING VIRAL!

The Wisconsin Institutes for Discovery (WID) are two unique entities, one private and the other public, housed in one stunning 300,000-square-foot facility with a unique design to facilitate collaborative research, education, and public outreach. **John Yin** leads one of five thrusts, Systems Biology, in the public part of WID. This group of researchers is exploring how frontiers of experimental and computational biology can advance and be enriched by evolutionary biology. Every human being is an ecosystem, in continuous exposure to a diversity of microbial cells and viruses present on our skin, in our guts, and in our tissues. "No organism is an island," says John. "We have known for a long time how bacteria and viruses can cause human disease, but the new data suggest they also have important and intriguing roles in promoting our health." John and his research team are developing new approaches to understand how viruses grow, spread, and evolve. If a virus particle is able to invade a living host cell, it reprograms the cell to turn it into a virus factory. Upon release by the cell, the progeny virus particles move by convection and diffusion to other cells, where they initiate further infections. A quantitative understanding of the material and energy flows of the infection process can highlight opportunities for therapeutic intervention. But, because infections start with a single viral particle, the biochemical reactions are "noisy" or "stochastic." **Jim Rawlings** brings his expertise in stochastic modeling into this effort to understand how viruses replicate, survive, mutate, and flourish. The ultimate aim is to promote human health through effective management of microbe-host interactions.

Beyond connecting scientists and engineers in the systems biology thrust, WID is reaching further “Forward,” connecting science to the arts and humanities, connecting ways of knowing to ways of understanding, and reflecting on the meaning of the new science on our humanity. Making connections from science to art is a particular interest of John, an accomplished cellist who studied at the Julliard School of Music and has performed with several symphony orchestras. Old friends of the department will be interested to know that our former chair, **Sangtae Kim**, returned to Wisconsin following stints in the pharmaceutical industry and government. Sang now serves as Executive Director of the Morgridge Institute for Research, the private half of WID.

## MRSEC AND NSEC: BIG IDEAS COME IN SMALL PACKAGES

Just renewed with \$18 million over six years, the NSF-supported Materials Research Science and Engineering Center (MRSEC) involves more than 40 faculty and 50 graduate students from disciplines ranging from chemical engineering to biology to medicine. The primary mission of the center is to understand and control the structure and dynamics of interfaces in a wide range of materials. Originally directed by **Tom Kuech** and now led by **Juan de Pablo**, MRSEC benefits from the participation of CBE faculty including **Nick Abbott**, **Paul Nealey**, **Sean Palecek**, **Jim Dumesic**, and **Dave Lynn**. The investigators work at the crossroads of advanced inorganic materials, polymers, and biological systems, connected by the common interest in heterogeneous interfacial phenomena. While the center is continuously evolving, at the current time MRSEC researchers are focused on three thrusts. The first seeks to create new semiconductors and is exploring new multi-element compounds through the manipulation of strain, dimensions, and deformability. The second thrust is organized around the study of molecular and electronic dynamics where carbon-based compounds meet inorganic compounds. “The work of our first two research groups will find direct applications in new technology for high-speed electronics, sensors, and solar cells,” says Juan. A third team will build knowledge about coupling structural, mechanical, and interfacial interactions in liquid crystalline materials through an emphasis on defect manipulation, nucleation, mechanical strain, and growth. Liquid crystals have the properties of both conventional liquids and solid crystals, with many phases in between. Through techniques such as confinement, nanoscale patterning, and the addition of multifunctional polymers that induce structural order in the liquid crystals, the group will create new classes of materials that have applications in separations technologies, drug delivery, nanoscale materials processing, and biosensors.

Research at the NSF-funded Nanoscale Science and Engineering Center (NSEC) focuses on templated synthesis and assembly at the atomic level. The center is directed by

Paul Nealey, and involves CBE faculty Juan de Pablo, Nick Abbott, and **Mike Graham**, as well as researchers across campus. NSEC researchers are directing the assembly of materials into functional systems and architectures through use of self-assembly, chemical patterning, and external fields. Researchers are developing new materials and processes for advanced lithography, in which self-assembled block copolymers are directed to adopt morphologies that advance the performance of nanomanufacturing processes. They are synthesizing biologically inspired organic nanostructures in which functional side chains display unique ordering, and exploring non-equilibrium processes for manipulating assembly of nanoscale objects.

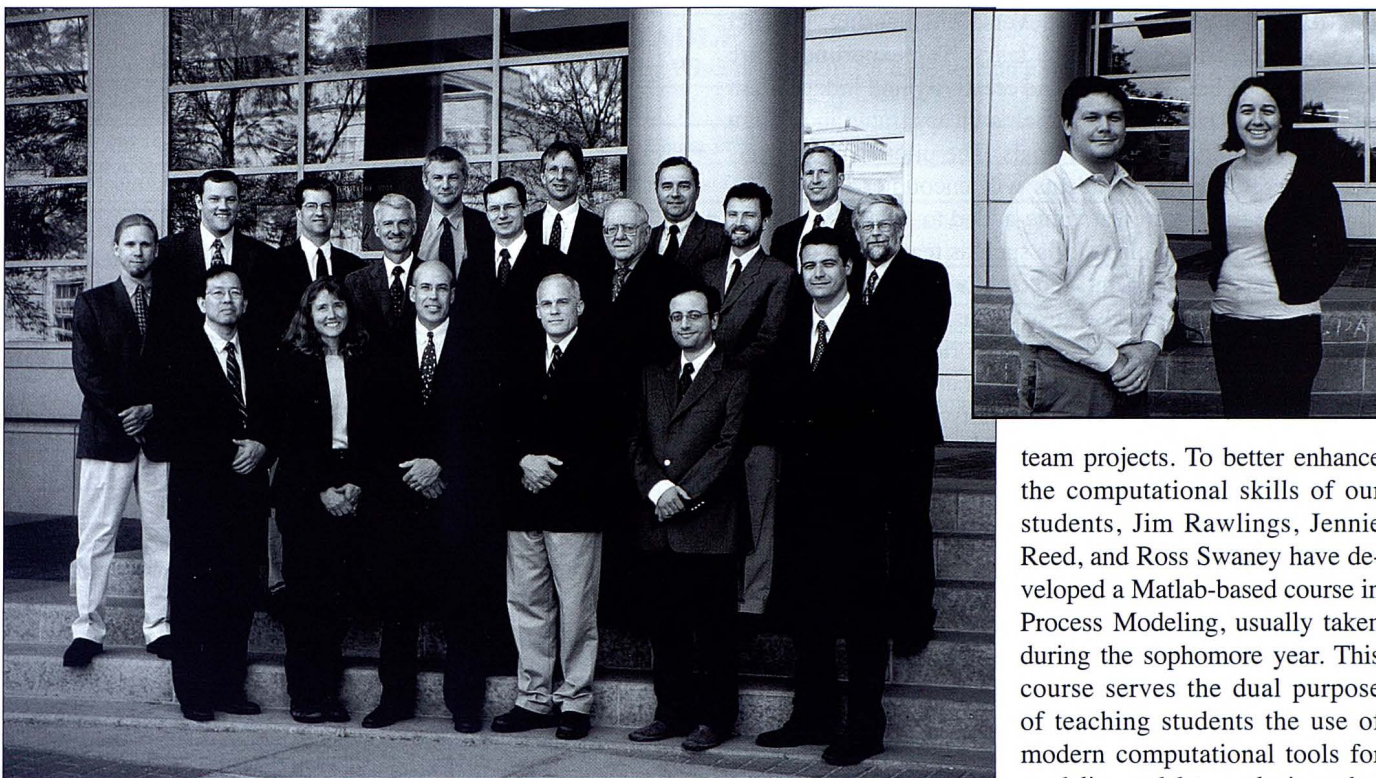
Not content just to move nanoscience and technology “Forward,” MRSEC and NSEC take seriously their responsibility to communicate with the public. Innovative K-12 outreach programs have led to the development of state-of-the-art lesson plans, instructional videos, and kits that are used throughout the world to educate the next generation of scientists and engineers. Over the last few years, the centers have distributed over 20,000 kits and reached 100,000 children!

## AND THAT’S NOT ALL...

The above gives just a taste of the larger multidisciplinary projects at Wisconsin. There isn’t room to describe all the exciting research going on in the CBE labs: We’ll just mention (in alphabetical order): **Dan Klingenberg’s** work on electrorheological and magnetorheological fluids for automobile parts like brakes, shock absorbers, and engine mounts, **Regina Murphy’s** studies on protein aggregation and its relationship to neurodegenerative diseases like Alzheimer’s, **Sean Palecek’s** design of strategies to control cellular signaling pathways and regulate cell function in human pluripotent stem cells, **Jim Rawlings’** efforts at improving the ability of networked utilities to manage resources and demand using model predictive control, **Thatcher Root’s** initiatives in developing new catalysts and processing strategies for environmentally benign manufacturing, **Eric Shusta’s** advances in developing in vitro models of the blood-brain barrier and innovative strategies for noninvasive brain drug delivery, and **Ross Swaney’s** work to develop field theories for macroscopic modeling and robust computational methods.

## BADGER ENGINEERS

Our undergraduate students survive one of the most grueling and rigorous curricula around: 133 credits of math, chemistry, biology, physics, liberal arts, and engineering. Despite, or maybe because of, the challenging curriculum, interest in chemical engineering among entering freshmen is very high. At Wisconsin, students need to apply for admission into a specific engineering department. Currently we are admitting 104 students each year. In order to accommodate the demand, we offer core courses every semester, and have expanded and



*Faculty in Wisconsin's Chemical and Biological Engineering Department. First row (left to right): John Yin, Regina Murphy, Juan de Pablo, Ross Swaney, Manos Mavrikakis, Christos Marevelias. Second and third row (left to right): Dave Lynn, Eric Shusta, Paul Nealey, Jim Rawlings, Nick Abbott, Sean Palecek, Dan Klingenberg, Charlie Hill (now retired), Jim Dumesic, Mike Graham, Thatcher Root, and Tom Kuech. Inset: our newest faculty members, Brian Pflieger and Jennie Reed.*

upgraded laboratories. Of course, we are interested in not just quantity of undergraduates but also quality of the undergraduate experience, and have recently implemented many innovations, with others in the works. Dan Klingenberg has collaborated with faculty from other engineering departments to develop and offer a "Grand Challenges" class to freshmen. This is one of three introductory engineering classes that freshmen can choose; students scrutinize the application of engineering solutions to the "grand challenges" facing society in energy, health care, environment, security, and quality of life. Plans are under way to expand this very popular class to allow non-engineering students to participate alongside engineers. Alternatively, freshmen can choose a design-based Introduction to Engineering, where they work as teams on projects generated by Madison-area clients. Several CBE faculty, notably Thatcher Root, have participated in this fun, hands-on class.

Other curricular innovations take advantage of technology. Regina Murphy has developed online animated and narrated presentations, quizzes, and interactive modules to accompany the introductory material and energy balance class. The online materials allow students to learn and review basic concepts, and free up classroom time for greater instructor-student interaction, in-depth analysis of more challenging problems, and

team projects. To better enhance the computational skills of our students, Jim Rawlings, Jennie Reed, and Ross Swaney have developed a Matlab-based course in Process Modeling, usually taken during the sophomore year. This course serves the dual purpose of teaching students the use of modern computational tools for modeling and data analysis, and of introducing students to concepts in process design, thermodynamics, kinetics, and transport that they will encounter in more depth later.

Upper-level electives provide opportunities for students to broaden and deepen their knowledge of particular areas of interest. Brian Pflieger has recently revived and updated a popular Biomolecular Engineering Laboratory, while Paul Nealey's course Plastics and High Polymers Laboratory provides students access to state-of-the-art equipment for polymer characterization. Tom Kuech, Nick Abbott, and Jim Dumesic share their respective expertise in Electronic Materials, Colloid and Interface Science, and Heterogeneous Catalysis. Thatcher Root has recently developed a new class in Energy and Sustainability, and also offers an undergraduate seminar-type class called Chemical Engineering Connections, where students explore chemical engineering topics that appear in the headlines.

## **SUMMER LAB (AKA 'CHEM-E BOOT CAMP')**

One of the most distinctive ingredients in our undergraduate curriculum is CBE 424 Unit Operations Lab, better known as Summer Lab, an intensive 5-week, 5-credit course that students can complete in Madison, or in international locations (currently Oviedo, Spain, or Vienna, Austria). The formal experiments involve distillation, heat transfer, humidification, pumps, and reactors. The larger portion of the lab time is spent on informal experiments that challenge students through

new-technology exploration, reverse engineering, product development, and optimization tasks. The experiments are not “scripted” but rather demand creativity and independent initiative as students construct their own apparatus and design experiments to achieve their goals. The pilot-scale projects closely resemble what students will encounter in industry. This course provides great value-added to employers of our students by strengthening skills such as teamwork, communication, time management, and creativity. Succinct oral and written communication also are emphasized, with memos favored over full reports, to reflect real-world practices. Students work with a variety of “bosses” for their different projects, and the diverse staff includes visiting faculty from abroad, retired practicing engineers, and UW-Madison faculty to provide a variety of perspectives, background, and expertise. Awards are given to pairs of students who exhibit the best teamwork and the most creative solutions. In a recent CBE alumni survey, one responder commented:

“As of your first day on the job, employers don’t care what school you went to, how your grades were or how smart you think you are. They care that you are able to work on a team, solve problems, and finish projects quickly and well. They also care that you bring a professional attitude to work. CBE 424 demanded all of these things.”

We’ve collected some other comments about Summer Lab from students in Table 1.

## BUSY BADGERS

Not content to spend all of their time in the lab or the library, undergraduate students at UW participate in an enormous variety of extracurricular activities. In any given year, about 100 students are conducting undergraduate research projects, 30 students are participating in 6-month industrial co-op experiences, and three students are studying abroad. Students participate in college activities from the Schoofs Prize for Creativity to the Burrill Technology Business Plan Compe-



Graduate students from Nick Abbott’s group examine nanostructured materials.

<b>TABLE 1</b> <b>Student Reflections on Summer Lab</b>
This course gave practicality to the other coursework (book stuff).
This course simulated real work more than any other. It was very focused and allowed the student to consume themselves in something for a period of time.
I think learning how to solve the problem was pretty cool. The frustration I had with the course was the difficulty in building things. I do similar things all the time in my job, but I have a well-stocked storeroom with nuts and bolts and screws and fasteners of all types plus I can order anything I need on the Internet, while summer lab was an exercise in scavenging.
While very intensive, to say the least, that class alone provided enough practical application of the CHE concepts I learned to, and I quote, “stun” various interviewers. They were very impressed that independent projects, especially nine of them in five weeks with write-ups, were undertaken in undergraduate courses.
Teamwork was another aspect that was learned—it did prepare me for the array of people that you have to form teams with in the professional world.
I took mine in Oviedo and really enjoyed the chance to study and live temporarily in a foreign country and still study in English.
Very hands-on and met awesome people from Clemson in Vienna. I am still friends with them and one is my boyfriend.
Its only value was as a personal test of endurance.
Once you accomplish this course, you can get through almost anything.
There’s some sense of pride that comes in finishing it, as well as some sense of “you should have to do it since I did!”
Pure torture.

tion to Engineering Expo—a three-day event run entirely by students that brings more than 10,000 visitors to campus.

Introduced in 2007, participation in iGEM, (international Genetically Engineered Machines) is increasingly popular, as student teams from universities around the world compete to design, conduct, and communicate experimental research projects in the field of synthetic biology. Teams receive a set of DNA molecules, called “biobricks,” that they have to assemble into functional devices. The 2011 UW-iGEM team investigated the use of biosensors to quantify two biofuels, ethanol and alkanes, using red fluorescent protein as a signaling device. To improve the sensitivity and dynamic range of these *E. coli*-based biosensors, the team constructed an operon of genes for use in an iterative selection process. Once optimized, the biosensors will be used to screen libraries of bacteria in search of strains that yield high levels of biofuel. At press time we learned that the team won a gold medal in a regional competition and was invited to present their work at the iGEM World Finals.

## PUTTING PEN TO PAPER

Wisconsin CBE faculty have a penchant for putting pen to paper (fingers to keyboard?). Table 2 shows a list of some of the books authored by past and present members of our

**TABLE 2**  
**Books Authored or Co-authored by Wisconsin Chemical Engineering Faculty**

Author	Title	Year
O.P. Watts	Laboratory Course in Electrochemistry	1914
O.A. Hougen and K.M. Watson	Industrial Chemical Calculations	1931, 1936
O.A. Hougen and K.M. Watson	Chemical Process Principles (vol 1) Material and Energy Balances	1943, 1954
O.A. Hougen and K.M. Watson	Chemical Process Principles (vol 2) Thermodynamics	1947, 1959
O.A. Hougen and K.M. Watson	Chemical Process Principles (vol 3) Kinetics and Catalysis	1947
O.L. Kowalke	Chemical Process Calculations	1947
W.R. Marshall, Jr., and R.L. Pigford	Applications of Differential Equations to Chemical Engineering Problems	1947
J.O. Hirschfelder, C.F. Curtiss, and R.B. Bird	Molecular Theory of Gases and Liquids	1954, 1964
F. Daniels and J.A. Duffie	Solar Energy Research	1955
R.B. Bird, W.E. Stewart, and E.N. Lightfoot	Transport Phenomena	1960, 2002
R.B. Bird and W.Z. Shetter	Een goed begin (A Contemporary Dutch Reader)	1963, 1971
E. J. Crosby	Experiments in Transport Phenomena	1961
D.F. Rudd and C.C. Watson	Strategy of Process Engineering	1968
W.H. Ray and J. Szekeley	Process Optimization	1973
D.F. Rudd, G.J. Powers, and J.J. Sirola	Process Synthesis	1973
E.N. Lightfoot	Transport Phenomena and Living Systems	1977
J.A. Duffie and W.A. Beckman	Solar Energy Thermal Processes	1977
E.E. Daub, R.B. Bird, and N. Inoue	Comprehending Technical Japanese	1975
P.M. Berthouex and D.F. Rudd	Strategy of Pollution Control	1977
C.G. Hill	An Introduction to Chemical Engineering Kinetics and Reactor Design	1977
R.B. Bird, R.C. Armstrong, and O. Hassager	Dynamics of Polymeric Liquids (vol 1) Fluid Mechanics	1977, 1987
R.B. Bird, O. Hassager, R.C. Armstrong, and C.F. Curtiss	Dynamics of Polymeric Liquids (vol 2) Kinetic Theory	1977, 1987
J.A. Duffie and W.A. Beckman	Solar Engineering of Thermal Processes	1980, 1991
W.H. Ray	Advanced Process Control	1981
W.Z. Shetter and R.B. Bird	Reading Dutch	1985
E.E. Daub, R.B. Bird, and N. Inoue	Basic Technical Japanese	1990
S. Kim and S.J. Karrila	Microhydrodynamics: Principles and Selected Applications	1991
J.A. Dumesic, D.F. Rudd, L.M. Aparicio, J.E. Rekoske, and A.A. Trevino	The Microkinetics of Heterogeneous Catalysis	1993
B.A. Ogunnaike and W.H. Ray	Process Dynamics, Modeling, and Control	1994
N. Phan-Thien and S. Kim	Microstructures in Elastic Media: Principles and Computational Methods	1994
J.B. Rawlings and J.G. Ekerdt	Chemical Reactor Analysis and Design Fundamentals	2002
R.M. Murphy	Introduction to Chemical Processes: Principles, Analysis, Synthesis	2007
W.E. Stewart and M. Caracotsios	Computer-Aided Modeling of Reactive Systems	2008
J.B. Rawlings and D.Q. Mayne	Model Predictive Control: Theory and Design	2009

department. This impressive list includes some texts that have revolutionized the teaching and practice of chemical engineering, pushing the field “Forward.” But did you know that **Bob Bird** has co-authored several books on Japanese and Dutch?

Recent textbook efforts include the 2nd edition of *BSL* (42 years after the first!), **Jim Rawlings’** book (with co-author **John Ekerdt**) that brings a new, mathematical/network approach to chemical kinetics, and Regina Murphy’s text with



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Win or lose, the Wisconsin Badger football team draws a large, enthusiastic crowd to Camp Randall.

a modern, design-based approach to material and energy balances. Also in the works is the text *Chemical, Biological and Materials Engineering Thermodynamics*, co-authored by Juan de Pablo and UW alumni **Jay Schieber**, and a 2nd edition of **Charlie Hill's** best-seller, *An Introduction to Chemical Engineering Kinetics & Reactor Design*.

Those of you who still have nightmares about those grueling homework sets on transport phenomena will be happy to learn about a new text now in the works. Dan Klingenberg is co-author, with Bob Bird of a new book, *Introduction to Transport Phenomena*, more in tune with the level of mathematical understanding of typical undergraduates. The new edition brings in Dan's years of experience in the classroom in our one-semester junior-level transport course, along with his research in rheology and his industrial consulting experiences. BSLK will re-arrange the presentation of shell balances, add missing steps in many examples and derivations, delete some of the most advanced concepts (those infamous Class C and D problems), and add chapters on dimensional analysis.

## MADISON: 76 SQUARE MILES SURROUNDED BY REALITY

The University of Wisconsin campus is situated smack dab in the middle of the city of Madison, a lively college town plus state capitol. You can argue about the state's choice of milk as its official beverage while enjoying a pitcher of Wisconsin's unofficial state beverage at the Union Terrace and watching the sunset over Lake Mendota. State Street is the pedestrian thoroughfare, lined with cafes, restaurants, and shops, that links Bascom Hill at the center of campus with the Capitol Square. There are plenty of opportunities for music and theater, both on campus and in the beautiful Overture Center for the Arts. Outdoor activities abound; bicycling the rolling hills of the surrounding farmland is particularly popular. Winter brings out the ice fishermen, ice sailors, hockey players, and cross country skiers. Badger athletics keep sports fans happy. And at every football game there is the opportunity to try out the polka when the marching band plays "Roll out the barrel!" □