Department of Chemical and Biomolecular Engineering 2007 Annual Report

THE UNIVERSITY of TENNESSEE
COLLEGE of ENGINEERING

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Department of Chemical and Biomolecular Engineering
2007 Annual Report

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Department Head's Message

Recent advances in life sciences and nanotechnology, as well as the looming energy crisis, have brought chemical engineering education to the threshold of significant changes. The Department of Chemical and Biomolecular Engineering (CBE) at the University of Tennessee, Knoxville (UTK) is transitioning to embrace and fully utilize these changes to meet global challenges in health care, the environment, renewable energy sources, national security and economic prosperity.

New demands on chemical engineering graduates, such as cross-permeation of ideas from evolving fields of biology, medicine and sustainability have provided the motivation for revision of our education research foci with an emphasis on biological systems and micro- and nano-structured materials, as well as sustainable energy. In early 2007 we adopted a new name, Department of Chemical and Biomolecular Engineering, to reflect significant changes in our program.

Full implementation of this new paradigm requires willingness to cross boundaries in our research and teaching programs. We are instituting innovative partnerships with other disciplines at UT, such as medical, life and physical sciences, as well as with the College of Business Administration.

Close collaboration with Oak Ridge National Laboratory (ORNL) through the Joint Institutes of Advanced Materials (JIAM), Biological Sciences (JIBS) and Computational Sciences (JICS) provide our students opportunities to use state-of-the-art supercomputers and obtain access to the Spallation Neutron Source (SNS), a one-of-a-kind facility providing the most intense pulsed neutron beams in the world.

In addition to joint ventures with ORNL, we have also established strong collaborations with two centers of excellence on the UTK campus, namely the Institute for Sustainable and Secure Environment (ISSE) and the Sustainable Energy Education and Research Center (SEERC), to provide our students world-class research and educational opportunities in the sustainable energy and technology arena.

I hope this brief overview has detailed the critical issues of this exciting transitional time in our department. Please offer us your support as we begin this crucial and timely transition, in which we strive to educate students for leadership roles in vital future technologies.

Bamin Khomami

Armour T. Granger and Alvin & Sally Beaman Distinguished Professor and Head of Chemical and Biomolecular Engineering

Dr. Bamin Khomami

The Power of Collaboration

Sustainable energy seems to be the new buzzword in both research and education on college campuses across the United States. At the University of Tennessee, Knoxville (UT), significant changes in the Department of Chemical and Biomolecular Engineering (CBE) have helped shape what the future of energy will look like. Within CBE, researchers work on three prongs of sustainable energy: photovoltaics, bio-fuels and fuel cells. Current research projects include inorganic and hybrid polymeric-biological photovoltaic materials; polyelectrolyte membrane hydrogen fuel cells; and hydrogen generation via water splitting.

Solar energy has long been touted as an alternative energy, but with high costs and low efficiency. Silicon-based solar cells, first introduced in 1954 by Bell Labs, use an exorbitant amount of labor and energy when produced, which end up costing the consumer a fortune. Dr. Bamin Khomami, Armour T. Granger and Alvin & Sally Beaman distinguished professor and head of CBE, works to improve photovoltaic efficiencies and thinks that within 10 years, worldwide consumption could jump by an order magnitude.

"Compared to fossil fuels technology, photovoltaic technology is in its infancy, but advancing at a rapid pace," said Khomami, who works on development of photovoltaic films created from specifically tailored semiconducting nanoparticles and coatings. "Photons contain energy that corresponds to different wavelengths of light," said Khomami. "Only photons of the right energy can excite electrons in a given system, which then flow to create an electrical current." Nanoparticles can be tuned, making them photoactive in different ranges of light and attractive prospects for researchers. "We are currently collaborating with Professor Biswas from Washington University to develop a simulation guided single-step flame aerosol reactor for deposition of semi-conducting nanostructured films that allows rigorous control of film thickness, morphology, composition and crystallinity and in turn, photovoltaic efficiency," said Khomami.

Hydrogen is produced using green algae and cyanobacteria by separating the photosynthetic protein complexes and enzymes from the cells and suspending them in solution.

Currently, Khomami, along with colleagues in the Departments of Biochemistry and Cellular and Molecular Biology (Dr. Bruce) and Chemistry (Drs. Dadmun and Mays) at UT, is working to overcome a significant obstacle in the production of commercially relevant polymeric photovoltaics - the lack of a fundamental understanding of the relationship between the morphology and interfaces that exist in multi-component polymer systems to the resultant exciton dissociation, charge conduction and ultimate device efficiency. By incorporating biological complexes, Khomami hopes to develop novel polymer photovoltaics with controlled morphologies in order to address this shortcoming.

"Incorporation of the biological complex at the biphasic interface will provide a dramatic improvement in the exciton dissociation process and thus provide a clear mechanism to improve device efficiency," said Khomami. "The use of diblock copolymers provides a robust method to control the morphology of the result photovoltaic material." Researchers are faced with surmountable challenges in this process, including developing conducting polymers that microphase separately into traditional diblock morphologies and developing strategies to guide biological complexes to the biphasic interface to realize their potential of optimizing exciton dissociation. "The project plan is designed to address these hurdles while creating a material that optimizes the device efficiency by controlling the morphology and interfaces and simultaneously providing fundamental information to enable the reproducible and efficient production of the next generation of photovoltaic materials created from multi-component conjugated polymer systems," said Khomami.

Dr. Brian Edwards, associate professor and associate head of CBE, and Drs. David Keffer and Stephen Paddison, associate professors in CBE, also play a significant role in the sustainable energy arena through their work on proton transport in proton exchange membrane (PEM) fuel cells.

"The idea is that it doesn't matter if you're generating energy for a power plant, home or car, all these processes create CO_2 and contribute to the main cause of global warming," said Keffer. "We need to find alternative ways of generating power and relevant to this theme of sustainable energy research in the university is the work we're doing with fuel cells."

In a fuel cell, hydrogen enters and is split into protons and electrons by a platinum catalyst. Electrons are carried off to do electrical work, and the protons have to complete the circuit by being transported through a membrane separating the electrodes. But for over 40 years, researchers have been stumped as to how the protons move through the electrode-electrolyte interface. Keffer, Edwards and Paddison are performing multiscale simulations to elucidate the mechanism of proton transport and nanostructure formation in PEM fuel cells.

"We're going to have to start thinking differently about how we make energy because we can't make it like we are now," said Dr. Paul Frymier, associate professor in CBE whose forward-thinking idea of energy production is to use plants for energy.

For billions of years, plants have transformed sunlight into energy through photosynthesis. Frymier and Dr. Barry Bruce, professor of biochemistry and cellular and molecular biology and adjunct professor in CBE at UT, believe this natural process can be used to create energy efficiently. "I've always been curious about a way to produce energy sustainably," said Frymier whose research focus is on in vitro (cell-free) systems for producing hydrogen because lots of energy is invested in sustaining enough live algae to produce hydrogen. Frymier also concentrates on engineering and optimization of photosynthetic routes to biohydrogen.

Whether processing spinach, PV films or proton exchange membranes, CBE researchers are contributing to the future of sustainable research and development in the energy sector.

"There's more to sustainability than energy," said Bruce. "It's never been part of the equation, but we have to change the energy dimension of the production process. We're trying to create a paradigm shift in how engineers are trained. They have not put sustainability in their equations, and I believe the new paradigm of engineering will have to address more complex parameters than the typical engineer usually does."

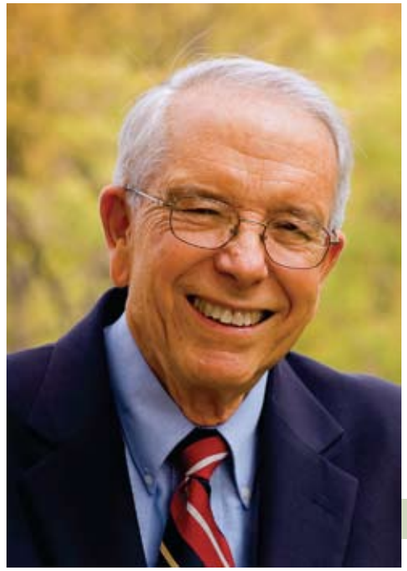
A Legacy of Excellence

Fifty years after completing his doctorate in chemical engineering at the institution he has since called home, the University of Tennessee's John Prados is being recognized for a lifetime of achievement in his field.

Prados, professor emeritus of chemical and biomolecular engineering and former UT vice president for academic affairs, has been named the recipient of the Lifetime Achievement in Chemical Engineering Pedagogical Scholarship Award from the American Society of Engineering Education (ASEE). The award is regarded as the society's highest honor for a chemical engineer. He received the award at the ASEE conference in Honolulu in June 2007.

The recognition reflects Prados' extensive work to change the fundamentals of engineering education, making it more focused on how students apply their knowledge, rather than just the number of hours they spend in scientific and technical studies.

Prados' entire career has been spent at UT, except for periods of research at Oak Ridge National Laboratory (ORNL) and a three-year stint in the 1990s with the National Science Foundation (NSF), through which he worked with engineering education programs across the country.



Dr. John Prados

In 1969, Prados was named as associate dean of the College of Engineering, and in 1971 he moved to UT administration as dean of admissions and records. Two years later, he was designated as vice president for academic affairs.

Prados also served as acting chancellor for UT-Knoxville and UT-Martin, and was the acting director for the UT Space Institute's Energy Conversion Division. Prados also served as department head for the chemical engineering department from 1990 until 1993.

Beginning in the 1970s, Prados worked with the Accreditation Board for Engineering and Technology (ABET), the organization that accredits engineering programs around the country. This experience spurred his desire to bring change to how engineers are educated.

"It became obvious to me that things needed to be fixed," said Prados. "We were very strong in math and science, but we needed to help students put engineering in the context of economic, social and environmental realities."

Prados' extensive background in education allowed him to view both the positives and negatives of traditional engineering education, and he determined that a broader focus was necessary as a critical component of changing engineering curricula.

"Math and science alone will not produce a device that is environmentally sound and aesthetically pleasing, for example," he said. "We must help students recognize the implications of their work."

Prados was a member of the original Basic Engineering Renovation Team, a group commissioned by the late COE Dean Jerry Stoneking in 1996 to create improvements in the freshman engineering curriculum. The college's Engineering Fundamentals Division (EFD) was established through the initiative and continues today as one of the most successful freshman engineering programs in the country. By helping focus engineering education on project-based learning, Prados' influence can be felt in engineering classrooms both at UT and across the country.

Another element of Prados' legacy is the impact of his time as the editor of the *Journal of Engineering Education*. In that position, which he occupied from 1995 to 2001, Prados helped bring a greater level of scholarly rigor to the field of research in engineering education, which helped elevate the field's stature in the larger engineering community.

"John has provided many years of great service to us at UT and to our colleagues in engineering education around the world," said Way Kuo, dean of UT's College of Engineering. "He's been a dedicated and tireless role model for countless faculty and students."

In spite of his official retirement in 2001, Prados continues to be active, teaching courses at UT as well as consulting with other colleges and universities in the United States and abroad on methodology to improve their engineering education programs.

AIChE Student Chapter Provides Many Valuable Opportunities

Students in the Department of Chemical and Biomolecular Engineering (CBE) at the University of Tennessee (UT) have the opportunity to join the American Institute of Chemical Engineers (AIChE), the world's leading organization for chemical engineering professionals, with more than 40,000 members from 93 countries.

Started in 1908, AIChE helped establish the discipline of chemical engineering and set the foundation for a constantly evolving and vital profession. More than 150 student chapters exist across the United States and provide resources for networking with chemical engineering majors and practicing engineers. Student chapters also provide information about mentoring opportunities, student conferences, scholarships and career opportunities.

University of Tennessee, Knoxville AIChE 2008 officers are Jared Johnson, president; Bradley Harris, vice-president; Nickyla Alliowa, secretary; and Kristen Dobrodziej, treasurer. Dr. David Keffer, associate professor, is the group's faculty advisor.

Nine students represented the CBE department at the 2007 Southern Regional AIChE meeting hosted by the University of South Carolina. From left to right: Ian Morris, Peter Haddix, David Keffer (chapter advisor), Matt Milazzo, Kyle Mack, Anne Wells, Brian Long, Brad Harris, Heath Johnson and Sarah Kyker (2007 chapter president).

Outstanding Faculty Member Dr. Brian Edwards (left) with researcher Bangwu Jiang

The Big Picture

When Brian Edwards was 9 years old, his home chemistry set was his favorite toy.

"I had a lot of fun with it, but I cannot say the same for my parents" said Dr. Edwards, who is currently associate department head and associate professor of chemical and biomolecular engineering at the University of Tennessee.

Edwards started down the path of chemical engineering at the University of Illinois, where he received his B.S. in 1986. His interest in chemistry and chemical processes was what brought him to chemical engineering.

"I wanted to be a chemist at first," said Edwards, "but my advisor told me I would make at least 40 percent more salary per year as a chemical engineer. Although I did not then understand the distinction between the two fields, that was enough for me at the time and I switched majors. Only later did I learn that choosing chemical engineering was much more than planning a career path."

After receiving his Ph.D. in chemical engineering from the University of Delaware in Newark in 1991, Edwards decided his interests and abilities were geared toward academic pursuits.

"I liked interacting with students and had ample opportunity to do so both at Illinois and Delaware as a teaching assistant," said Edwards. "Furthermore, the academic freedom to pursue the engineering problems that interested me, as opposed to working on problems that someone else had mandated, also appealed to me."

Edwards' primary research focus is at the interface of thermodynamics and fluid dynamics, especially as applied to the polymer processing operations used in the manufacture of semi-conductors, plastics, surgical devices and a myriad of other products used every day by billions of consumers worldwide. In his book, *Thermodynamics of Flowing Systems with Internal Microstructure*, co-authored with Dr. Antony N. Beris, he laid out a methodology for describing dynamical complex fluid processes from the ground up; this book has been cited over 350 times by other researchers.

Sustainable energy is another area in which Edwards works, in collaboration with other professors in the department; in particular, the conversion of hydrogen gas into electrical power.

"I like to think about the big picture," said Edwards. "Eventually, fossil fuels will dry up, maybe sooner than we expect. Alternative forms of energy are necessary, and hydrogen as a fuel has potential to impact energy use across the globe."

Fuel cells are part of this big picture for Edwards, who leads the Computational Materials Research Group with Dr. David Keffer, associate professor of chemical and biomolecular engineering at UT. In a fuel cell, hydrogen enters and is split into protons and electrons by a platinum catalyst. For over 40 years, researchers have tried to understand how protons move through the electrode-electrolyte interface of fuel cells. With help from a Department of Energy grant, Edwards hopes to discover the answer through a computer model membrane he and Keffer created at the molecular level to look at the vehicular and structural diffusion that takes place with the cells.

Edwards has also been recognized for his professionalism in teaching and research. In 2003, he was awarded the College of Engineering Outstanding Faculty Advisor Award and the Departmental Outstanding Teacher award. Four years later, Edwards was named a 2007 COE Research Fellow and received the Tom and Ruth Clark Award for Excellence in Chemical Engineering Teaching.

The primary reason Edwards joined the faculty at UT was that the College of Engineering and the Department of Chemical and Biomolecular Engineering, in particular, were poised for long-term and rapid growth.

"I chose to teach at UT's College of Engineering because I wanted to be part of building an imminent and sustainable national program of education and research in the chemical engineering profession, rather than merely another cog in the machine of an already well-established institution."

CBE Department Maintains Continuous ABET Accreditation

The Department of Chemical and Biomolecular Engineering (CBE) was recently accredited for six more years through the Accreditation Board for Engineering and Technology (ABET), a non-governmental, peer-review body that certifies quality in engineering educational programs at the university level on a nationwide basis. Accreditation is not a ranking system, but instead ensures that rigorous standards of education, ethics, professional development and lifelong learning are met. It also provides guidance to parents and students on which programs meet established quality standards.

"In general, programs not certified by ABET are considered not to have a standard minimum quality," said Dr. Masood Parang, associate dean for student affairs in the College of Engineering. "Most employers are aware of the accreditation and would like to hire only graduates of the ABET-accredited engineering programs and schools."

ABET accreditation standards are set by professionals through collaborative efforts of many technical and professional societies. Although ABET accreditation is voluntary on the part of the institution, accreditation helps students and their parents choose quality college programs, and enables employers to recruit well-prepared graduates. Accreditation also gives colleges and universities a structured mechanism to assess, evaluate and improve the quality of their programs.

Outstanding Graduate Student Jared Fern

Real World Solutions

When Jared Fern started college at Middle Tennessee State University, he wanted to become a medical doctor. While studying biology and chemistry, however, Fern discovered a passion for chemistry and its applications to the real world.

"The primary thing that interests me about chemical engineering is the connection of molecular interactions to real world problems," said Fern, who received his B.S. in chemical engineering from UT in 2003. "I chose to study at UT because it has one of the premier programs in the state for chemical engineering."

Fern, originally from Columbia, Tenn., is currently working on his Ph.D. in chemical engineering. He is a member of the American Institute for Chemical Engineers (AIChE) and won the 2007 Jim and Sandra McKinney Outstanding Graduate Student Award.

"My research interests are performing molecular simulations of vapor-liquid equilibrium and other complicated systems," said Fern, who plans to obtain a postdoctoral position at a national laboratory. Fern has focused on the investigation of vapor-liquid equilibrium (VLE) by molecular simulation, specifically molecular dynamics, and has recently addressed the limitations of current molecular simulation methods for measuring VLE. Along with his departmental advisors, Dr. William Steele, research professor, and Dr. David Keffer, associate professor, Fern has invented a new self-consistent method to measure VLE using Voronoi Tessellations and has applied this method to industrially relevant compounds, such as ethanol and ethylene glycol.

"The method utilizes Voronoi Tessellations to determine the volume of every molecule and atom in the simulation cell," said Fern. "By coupling simple statistical parameters, such as the average molecular volume and variance of the molecular volume, one can determine the individual phases in a multiphase molecular simulation."

"Jared has not only become an expert in molecular dynamics simulation, but also has taken a leadership role in training incoming students and researchers in the UT Computational Materials Research Group," said Keffer. "Jared has embraced each task offered to him, ranging from setting up experimental equipment in the thermophysical properties lab, to running the molecular simulations that comprise the core of his research, to performing continuum-level models in support of other research projects outside the department. He is an extremely talented and reliable person, and it has been a pleasure to have been part of his growth as a researcher during his time as a graduate student."

Making an Impact

It was chicken fat that first sparked Robyn Chaplin's interest in chemical engineering when, as a high school junior in Nashville, Tenn., she read an article on using chicken fat to heat buildings at the University of Georgia. "I thought it was an interesting solution to many problems, like foreign energy dependence and overflowing landfills," said Chaplin. "I had always excelled at math and science, but wanted to study something where I would have an impact on human life. Engineering was the perfect fit."

Originally from Largo, Fla., Chaplin, a senior in chemical engineering, is interested in renewable energy and plans to put her technical skills to work in an industrial setting. "I like the versatility of chemical engineering. My degree will provide a strong foundation for working within many industries that affect daily life," said Chaplin. "I have found I enjoy manufacturing and want to work at a plant that makes cellulosic ethanol, biodiesel, or something similar."

As a high school senior, Chaplin visited UT on Engineer's Day and was fascinated with the concrete canoes, robots playing ping-pong and a hybrid car built by students. "Seeing math and science in action solidified my desire to be an engineer," said Chaplin, who was impressed by freshman Engineering Fundamentals at UT, a program recognized nationally for its excellence.

One of Chaplin's most memorable experiences in the chemical engineering department was working on the "ChemE Car" project. "As a group of four, we attempted to fix a model car to be powered by a hydrogen fuel cell via a reaction of magnesium and hydrochloric acid. It seemed simple, but there were many challenges to overcome. The car drifted to one side and would not go a reproducible distance, even with the same chemical input," said Chaplin. "The experience showed me that chemical engineering is not only theoretical, but a problem-solving discipline as well."

While at UT, Chaplin studied Spanish in Costa Rica during the fall of 2006. She also represented UT in the 2007 Nissan-World Wildlife Fund Environmental Leadership Program.

"The program was highly beneficial in that it showcased environmental efforts from many fronts," said Chaplin. "It solidified the fact that legal policy and conservation are not the only means of protecting the earth. Peoples' material needs can be met in a more sustainable manner and technical expertise is needed to achieve that goal, which encourages me to seriously pursue a career in biofuel production."

Outstanding Undergraduate Student Robyn Chaplin

Environmentally Friendly Energy

Dr. Paul Frymier, associate professor of chemical engineering at the University of Tennessee, thought he wanted to design airplanes for a living, so he initially obtained a degree in aerospace engineering. However, when it came to finding a job with a healthy impact on the environment, he was hard-pressed to find one.

"Sustainable energy is something I've always been interested in," said Frymier. "As a kid I used to do science experiments with photovoltaics and was always interested in the 'how' of energy."

After completing both bachelors and master's degrees in aerospace engineering from North Carolina State University in 1985 and 1987, respectively, Frymier took a break from the books and headed into the Peace Corps, where he spent two years teaching high school-aged students and trying to implement educational and food production strategies to increase the quality of life of people in Gambia, West Africa.

"I learned two things in the Peace Corps," said Frymier. "One, the value of energy and sanitation in developing countries; and two, standard of living and quality of life are not always the same thing. If people are able to provide clean water and energy for food and medicine storage, it improves their quality of life. More televisions probably do not."

While in the Peace Corps, Frymier read books on clean water supply and sustainable energy technologies, and upon his return to the States, began looking for graduate programs that applied his fluid transport background to sustainable technologies.

Outstanding Faculty Member Dr. Paul Frymier (left) with graduate student Mehrsa Raeiszadeh

"Unfortunately, I was unable to find one," said Frymier, who wanted more than advanced wind turbine designs. He eventually decided to enroll at the University of Virginia and apply his engineering background to rehabilitation engineering. However, said Frymier, "The fit wasn't right. The problems were important and made a positive impact on people's lives, but I did not find the work to be something I was personally excited about."

Meanwhile, a friend suggested he might find something interesting in chemical engineering. "Initially I thought to myself, 'But I haven't really enjoyed chemistry,'" said Frymier. Luckily, the graduate program advisor in chemical engineering appreciated his background in transport. "A half hour later, I was majoring in chemical engineering on a full assistantship with a healthy stipend." While in the first year of his Ph.D program, Frymier earned a fellowship through the Department of Energy to work on environmental remediation problems.

Frymier graduated from the University of Virginia in 1995 with a Ph.D. in chemical engineering and a desire to teach.

"Throughout my education and career, faculty are the people I have most admired," said Frymier. "I wanted to be a professor rather than a captain of industry because I believe faculty are genuinely interested in their research and want to solve problems to have a significant impact on people's lives. Professors are accepted as bona fide experts doing important work and respected for it. That's why I chose a teaching and research career."

And it seems Frymier found the right fit. Since he has been part of the faculty in the College of Engineering, Frymier has received the Leon and Nancy Cole Superior Teaching Award, 2007; the Departmental Outstanding Teacher Award, 2002, 2004 and 2006; and the Departmental Excellence in Teaching Award, 2004.

Frymier's early research at UT focused on two areas: mass and momentum transport and bacterial adhesion in environmental and biological systems and toxicity biosensors. He measured the characteristic properties of microbial interactions with solid surfaces to identify and quantify the mechanisms involved in the interactions. Simultaneously, he worked with graduate students to accurately and efficiently model microbial transport and remediation rates at contaminated waste sites. In his work on toxicity biosensors, he developed new hybrid sensor microorganisms and systems for monitoring aquatic toxicity.

However, the time finally came for him to apply his work at the interface of biology and engineering in the Department of Chemical and Biomolecular Engineering to the sustainable production of fuel. He is pursuing this goal through his work with algae, cyanobacteria and the production of hydrogen.

"Since I was a kid tinkering with photovoltaic cells glued to model cars, I've always been interested in alternative energy sources for transportation," said Frymier. "When looking for universities to work at, the thing that piqued my interest about UT was its close proximity to Oak Ridge National Laboratory and the on-campus Center for Environmental Biotechnology. The combination of campus resources and biological scientists and engineers coupled with the close relationship of UT and ORNL were major factors in my decision to settle in Knoxville."

Currently, Frymier's research focus is on in vitro (cell-free) systems for producing hydrogen because lots of energy is invested in sustaining enough live algae to produce hydrogen. Frymier also concentrates on engineering and optimization of photosynthetic routes to biohydrogen.

Frymier's children, Fionna Martin, 10, and Gareth Frymier, 8, remind him of the necessity of his research.

"There's a problem I want to be a part of solving," said Frymier. "I've seen the difference in the developing world, and I want to help out. My kids will be inheriting this planet, and I want to be part of the solution for future generations."

New Faculty Member Dr. Eric Boder

Standing Out from the Crowd

Dr. Eric Boder joined the Department of Chemical and Biomolecular Engineering (CBE) August 1, 2007. Boder received his B.S. in chemical engineering from Washington University in 1993 and continued to study chemical engineering at the graduate level at the University of Illinois, where he obtained both master's and Ph.D. degrees in 1996 and 1999, respectively.

Before coming to UT, Boder was assistant professor in the Departments of Chemical and Biomolecular Engineering and Bioengineering at the University of Pennsylvania. He completed his postdoc work at the National Jewish Medical and Research Center in Denver, Colo., in the Department of Immunology.

Boder's research interest is molecular bioengineering. He is currently exploring two biomolecular systems that demonstrate switching in response to environmental conditions. In one case, Boder hopes to engineer controllable molecular switches that regulate adhesion of cells or particles to surfaces under flow. In the second case, Boder and his research team are developing tools for engineering controllable membrane fusion. "Both of these systems have a potential role in drug delivery and nonviral gene transfer," said Boder. "In addition, my lab is working on novel ways to attach proteins to surfaces and to each other, which is an important issue in proteomics and bionanotechnology."

Throughout his academic career, Boder has stood out from the crowd and been recognized for his achievements. Boder received an NSF Graduate Research Fellowship from 1993-1996 and was a National Academy of Engineering "Frontiers of Engineering" Invitee in 2002. He also received a prestigious NSF CAREER Award in 2003 for his work titled "Biomolecular Engineering of Antigen Presentation: Development of an Interdisciplinary Research and Education Toolkit." He is a member of the AIChE, Society for Biological Engineering, The Protein Society and the American Chemical Society. Boder has over 18 refereed publications and holds four U.S. patents.

"UT is an institution on the rise in nearly every respect. A great vision of the future exists on this campus, in particular with respect to my own area of biomolecular science and engineering, and it is extremely exciting to join, and hopefully play a significant role, in the effort to achieve this vision," said Boder. "The collegiality of colleagues across campus, the partnerships with Oak Ridge National Laboratory and the excellent support of the administration create a nearly unparalleled opportunity to make a real impact through research and education. Living in beautiful East Tennessee is an added bonus."

An Opportunity to Contribute

Dr. Stephen J. Paddison joined the Department of Chemical and Biomolecular Engineering (CBE) August 1, 2007. Paddison, originally from Canada, comes to UT from the Department of Chemistry at the University of Alabama, Huntsville (UAH), where he was an assistant professor for three and half years.

"I choose CBE at UT for the opportunity to join a department with faculty members active in computational materials science and engineering research," said Paddison, who received his Ph.D. in physical and theoretical chemistry from the University of Calgary in 1996. "My research is both distinct and complimentary to theirs, and I saw the opportunity in CBE to contribute to common and new research thrusts with other members of the department and the nearby Oak Ridge National Lab."

Paddison's main focus of research is the polymer electrolyte membrane (PEM), which is used as the separator in low temperature proton exchange membrane (PEM) fuel cells. "My research continues to be in the general area of computational materials chemistry," said Paddison. "Understanding the properties and chemistry of materials at the molecular-level entails the application of a variety of methods including first principles based and statistical mechanical formulations."

Paddison was educated as a chemical physicist and has worked in industry and at the Los Alamos National Laboratory doing reservoir and materials engineering. "My interest in chemical engineering is not new," said Paddison. "For the past 11 years, my research has been in the area of PEM fuel cells with a specific focus on materials modeling."

Paddison was a visiting fellow at Fitzwilliam College, University of Cambridge in the summer of 2003 and a guest scientist at the Max-Planck-Institut für Festkörperforschung during the summer of 2004. He continues collaboration with both institutions in research involving experimental and computational studies of PEM fuel cell materials.

In 2002, Paddison received the Gold Quill Award from Motorola Inc., the mark of global distinction and the highest level of professional acknowledgement within business communication today. He also received the UAH Foundation Research & Creative Achievement Award in 2007. Paddison holds one patent, has over 50 publications and is the referee for a dozen different professional journals.

Paddison is a member of the American Chemical Society, the Electrochemical Society, The Canadian Society of Chemical Engineers and the International Society for Solid-State Ionics.

New Faculty Member Dr. Stephen Paddison

A Distinguished Role Model

Dr. Michael Harris knew nothing about engineering when a recruiter from Mississippi State University (MSU) visited his high school in Mound Bayou, Miss. Interested in majoring in chemistry with a minor in mathematics, Harris talked to the recruiter, who convinced him to major in chemical engineering since he was not too fond of taking numerous English classes.

"To my knowledge, there were no engineers in my hometown," said Harris. "I learned later that my high school principal had a degree in electrical engineering."

Once Harris settled into his classes at MSU, he became totally excited about chemical engineering and graduated with highest honors before choosing UT for his graduate studies.

"After graduating from MSU, I was hired by Dr. Charles Scott at Oak Ridge National Laboratory to work in the area of environmental control technology," said Harris. "The evening graduate program at UT through Oak Ridge Associated Universities was ideal for someone like me who could work by day at one of the premier national laboratories and receive a Ph.D. from a Tier I research institution at night."

While at UT, Harris focused on colloids and interfacial phenomena with special emphasis on silica nanoparticles, hydrous metal oxides by metal alkoxide hydrolysis sol-gel processes, electrodispersion processes and hybrid boundary element/finite element numerical methods for solving electrohydrostatics of pendant and sessile drops. He received his Ph.D. in chemical engineering from UT in 1992.

"My most memorable event at UT was the day I received my Ph.D. and my grandfather told me how proud he was," said Harris.

Harris has since received numerous national and local awards. In 2005, he received the AIChE Grimes Award for Excellence in Chemical Engineering, an award presented by AIChE's Minority Affairs Committee, which recognized his outstanding achievements as a distinguished role model for minorities. Harris was also honored at the Engineering Faculty Recognition Banquet at Purdue University, receiving the 2006 Mentoring Award. Other awards include the Martin Marietta Energy Systems Significant Achievement Award, 1994; an AIChE Teaching Award from the University of Maryland, College Park, 1997; and a prestigious NSF CAREER award in 1997 for a research program titled: "Electrohydrostatics, Electrohydrodynamics and Microstructural Evolution During Electrodispersion Precipitation."

"For over a decade, Harris has excelled as an effective teacher, researcher and administrator," said Dr. Brian Edwards, associate professor and associate head of the Department of Chemical and Biomolecular Engineering at UT. "His national recognition as a progressive, distinguished role model for minorities through the American Institute of Chemical Engineers 2005 Grimes Award for Excellence in Chemical Engineering is one reason our department is proud to call him an alumni."

Harris's current research interests include biotemplated synthesis of nanowires and nanometric metal particles for sensor applications; use of electrodispersion processes for the synthesis of calcium alginate microspheres for the controlled-release of drugs; theory and experiment of external field effects on particle deposition from an evaporating drop; electrohydrodynamics of free, pendant and sessile drops; and theory and experiment of electrokinetics in porous media.

Because of his desire to recruit and graduate students, Harris chose to teach and is currently a professor of chemical engineering and associate dean for undergraduate education at Purdue University.

"Teaching gives me the opportunity to accomplish my goals to attract more female and minority students to engineering," said Harris. "I like to encourage students who have great potential, but who lack confidence to excel in engineering. My greatest joy is to receive letters from students thanking me for encouraging them and challenging them to perform well in their engineering studies, and for encouraging them to go to graduate school."

Outstanding Alumnus Dr. Michael Harris

Renowned Lecturers Discuss Intriguing Engineering Issues

The CBE department hosted two distinguished lecture series this year.

Professor Robert C. Armstrong, Chevron Professor and Chemical Engineering Department Head at the Massachusetts Institute of Technology (MIT) presented "The Global Energy Challenge and MIT's Response" February 6, 2007, in the Science and Engineering Research Facility on the UT campus.

Armstrong addressed concerns about sustainable energy sources that will meet demands for quality of life and economic growth in both the developed and developing worlds. He illustrated MIT's response to these challenges.

Dr. James C. Liao was the special guest for the department's annual Troy C. Trotter Distinguished Lecture Series in Chemical Engineering. A pioneer in the fields of metabolic engineering, synthetic biology and systems biology, Liao is currently serving as the Vice Chair of the Chemical and Biomolecular Engineering Department at the University of California, Los Angeles.

Liao's topic was "Synthetic Biological Circuits," and his presentation involved a discussion of design approaches to engineer cellular networks at both genetic and metabolic levels.

The Troy C. Trotter Distinguished Lecture Series was established by the Trotter family to provide the CBE department with opportunities to invite nationally recognized experts in areas of interest to the field of chemical engineering to the University of Tennessee, Knoxville for the benefit of students, faculty and the local professional community. The series recognizes and honors Troy C. Trotter, who received a B.S. in chemical engineering from UT in 1947. Trotter retired as Director of Project Site Engineering for Y-12, K-25 and Oak Ridge National Laboratory (ORNL) in 1986.

Faculty Listing

Paul Bienkowski
Professor
Ph.D., Purdue University
Research areas: Thermodynamics; environmental biotechnology

Eric Boder
Associate Professor
NSF CAREER Award
Ph.D., University of Illinois
Research areas: Molecular biotechnology and bioengineering; protein engineering

Duane Bruns
Associate Professor
Ph.D., Univ. of Houston
Research areas: Process dynamics; control and automation

Robert Counce
Professor
Ph.D., Univ. of Tennessee
Research areas: Green engineering; process design; separations

David Keffer
Associate Professor
Ph.D., Univ. of Minnesota
Research areas:
Molecular modeling; confined fluids; separations; sustainable energy

Bamin Khomami
Granger and Beamon Distinguished Professor and Head
Ph.D., Univ. of Illinios-Urbana
Research areas: Transport properties of complex fluids; sustainable energy; multiscale modeling & simulation

Charles Moore
Professor Emeritus
Ph.D., Louisiana State
Research areas: Areas of distillation design; operation and control

Shengting Cui
Research Assoc. Professor
Ph.D., University of Virginia
Research areas: General molecular modeling of materials properties and fluid phenomena

Brian Edwards
Associate Professor and Associate Head
Ph.D., Univ. of Delaware
Research areas: Thermodynamics; fluid mechanics; molecular modeling

Paul Frymier
Associate Professor
Ph.D., Univ. of Virginia
Research areas: Engineering and optimization of photosynthetic routes to biohydrogen

Stephen Paddison
Associate Professor
Ph.D., Univ. of Calgary
Research areas:
Computational materials science as applied to fuel cell electrolytes and electrocatalysts

Simioan Petrovan
Research Assoc. Professor
Ph.D., Technical University Iasi, Romania
Research areas: Characterization (rheological in particular) and processing of polymers

John Prados
Univ. Professor Emeritus
Ph.D., Univ. of Tennessee
Research areas: Engineering education, with special emphasis on active, collaborative learning and teamwork

Tse-Wei Wang
Associate Professor
Ph.D., Massachusetts Institute of Technology
Research areas: Bioinformatics; organization and search in large databases; data mining

Superior Support

The Department of Chemical and Biomolecular Engineering's (CBE) support staff provides a number of significant services to the department. Several staff members have been with CBE for many years.

"We are very grateful to have such a wonderful and dedicated support staff," said Dr. Bamin Khomami, CBE department head. "They are the backbone of the department, and we value their service."

CBE staff members and the years of service include: *(left to right)* Larry A. Smith, technical specialist-mechanical systems, 18 years; Betty Frazier, administrative specialist I, 28 years; Stephen A. Stiner, technical supervisor, Electronics Shop, 33 years; Marva Anderson, accounting specialist II, 13 years; Amy M. Brewer, business manager, 2 months; Susan Seymour, administrative support assistant III, 8 years; H. Bradley Snyder, senior technical specialist-Electronics Shop, 1 year; and Douglas A. Fielden, technical supervisor-Mechanical Systems, 25 years.

Board of Advisors

The Department of Chemical and Biomolecular Engineering's Board of Advisors consists of a distinguished group of academics, business professionals and industrial leaders from noted universities and international corporations.

The purpose of the board of advisors is to ensure that the department is focused on its mission of education, research and service to the university and technical communities. The board meets once a year to examine and evaluate CBE's undergraduate and graduate curricula and to advise the department head and faculty with regard to these issues.

The board provides insight into the activities of peer departments at other universities and offers information about the requirements of relevant industries. The board also acts as a liaison between the department, the dean's office and university administration, providing a candid assessment of the department's strengths and weaknesses, as well as communicating the department's directions, goals and resource requirements.

Current members of the CBE Board of Advisors are:

Mr. Victor H. Agreda, director of the chemical development division at Eastman Chemical Company in Kingsport, Tenn. Agreda is a member of Tau Beta Pi, the American Institute of Chemical Engineers (AIChE), and is the Chair of the Eastman Acetyl Technology Council.

Dr. Robert Armstrong, deputy director of the Massachusetts Institute of Technology (MIT) Energy Initiative/Chevron at MIT in Cambridge, Mass. Armstrong is past president of the Society of Rheology and has served as head of the Department of Chemical Engineering at MIT. Armstrong has received numerous awards for his research and teaching contributions including the Warren K. Lewis and the Professional Progress Award of the American Institute of Chemical Engineers, and the Bingham medal of the Society of Rheology.

Mr. Bruce Combs is the global site logistics director, Base Plastics, for the Dow Chemical Corporation in Freeport, Texas. Combs, a University of Tennessee chemical engineering graduate, is the past president of the Society of Professional Engineers (SPE), South Texas section.

Dr. George Georgiou is the Joan and Keys Curry/Cullen Trust Endowed Chair and a professor in the Department of Chemical Engineering at the University of Texas-Austin. He is the recipient of the Marvin J. Johnson Award in Microbial and Biochemical Technology from the American Chemical Society and has received the Professional Progress Award for Outstanding Progress in Chemical Engineering from the American Institute of Chemical Engineers. He also received the University Cooperative Society's Research Excellence Award for Best Paper at UT-Austin and the E. Bergman Award from the US-Israel Science Foundation.

Mr. James B. Porter Jr. is the chief engineer and vice president of engineering operations at the DuPont Corporation, headquartered in Wilmington, Del. Porter, a University of Tennessee graduate, is a member of the Construction Industry Institute, the Engineer and Construction Contracting Associates and serves on the Board of Directors of AIChE.

Dr. Eric Shaqfeh is professor of chemical and mechanical engineering at Stanford University in Stanford, Calif. Shaqfeh is a Fellow of the American Physical Society and also received the American Society of Engineering Education (ASEE) Research Award, National Science Foundation Presidential Young Investigator Award, the American Physical society Francois Frenkiel award and the David and Lucile Packard Fellow in Science and Engineering.

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Outstanding CBE Students, Faculty and Staff Honored at Ceremonies

The CBE Department hosted its annual awards dinner Wednesday, April 25th, 2007. The following individuals were recognized at the event:

Student Awards

AIChE Service Award—Sarah Kyker
Dow Outstanding Junior—Nickyla Alliowe
Kenneth M. Elliott Outstanding Senior Award—Kristen Dobrodziej
Jim and Sandra McKinley Outstanding Graduate Student Award—Jared Fern
Most Exceptional Student Award—Robyn Chaplin
American Chemical Society Outstanding Senior Award—Hillary Holback
Alpha Chi Sigma Albert Cooper Award—Anne Wells

Faculty and Staff Awards

Outstanding Staff Member Award—Susan Seymour
Outstanding Advisor Award—Dr. Brian Edwards
Outstanding Teacher Award—Dr. Tse-Wei Wang
Chemical Engineering Excellence Award— Dr. Brian Edwards

AIChE Awards

AIChE Outstanding Award—Patrick Bowland
AIChE Outstanding Baccalaureate Award—Latoyia Thompson

College-wide Awards & Recognitions

Several CBE faculty and students were also recognized at the College of Engineering Honors Banquet, April 10, 2007.
Leon and Nancy Cole Superior Teaching Award—Dr. Paul Frymier
COE 2007 Research Fellow—Dr. Brian Edwards
COE 2007 Outstanding Faculty Member—Dr. Bamin Khomami
Eastman Chemical Company Chemical Engineering Scholar—Jeffrey Keith Clark II
College Ambassador—Christopher Otuonye

Published Journal Articles and Book Chapters

For the period of July 1, 2006 to June 30, 2007.

1. A comparison of simple rheological models and simulation data of n-hexadecane under shear and elongational flow, C. Baig, B. Jiang, B.J. Edwards, D.J. Keffer and H.D. Cochran, *J. Rheol.*, 50, 625-640 (2006).
2. Influence of aqueous/solid interactions on organic droplet shape in liquid/liquid/solid systems, S.A. Morton III, D.J. Keffer and R.M. Counce, *Separ. Sci. Technol.*, 40, 2515-2531 (2006).
3. Development of a three-stage system for wastewater toxicity monitoring. A design and feasibility study, S. Ren and P.D. Frymier, *Water Environ. Res.*, 78, 965-973 (2006).
4. Effect of ionic strength on oil Removal from Stainless Steel in the Presence of Ionic Surfactant, N. Davis, S.A. Morton, R.M. Counce, D.W. DePaoli and M.Z. Hu, *J. of Sep. Sci. Tech.* 41, 3313-3328 (2006).
5. Green Production of Hydrogen from Excess Biosolids Originating from Municipal Waste Water Treatment, B. Bagchi, J. Rawlston, R.M. Counce, J.M. Holmes and P.R. Bienkowski, *J. of Sep. Sci. Tech.* 41, 2613-2628 (2006).
6. Liquidus curves of NH_4NO_3 (aq) calculated from the modified adsorption isotherm model for aqueous alectrolytes, W.O. Rains and R.M. Counce, *J. of Sep. Sci. Tech.* 41, 2629-2634 (2006).
7. Utilizing green engineering concepts in industrial process synthesis, R.M. Counce and S.A. Morton III, chapter in *Sustainability Science and Engineering: Defining Principles*, M.A. Abraham (Ed), Elsevier (2006).
8. Turbulent channel flow of dilute polymeric solutions: Drag reduction scaling and eddy viscosity model, V.K. Gupta, C.F. Li, R. Sureshkumar and B. Khomami, *J. Non-Newtonian Fluid Mech.*, 139, 177 (2006).
9. Time-dependent simulations of non-axisymmetric patterns in Taylor-Couette flow of dilute polymeric solutions, D.G. Thomas, U.A. Al Mubaiyedh, R. Sureshkumar, and B. Khomami, *J. Non-Newtonian Fluid Mech.*, 138, 111 (2006).
10. Influence of rheological parameters on polymer induced turbulent drag reduction, C.F. Li, R. Sureshkumar and B. Khomami, *J. Non-Newtonian Fluid Mech.*, 140, 23 (2006).
11. Pattern formation in Taylor-Couette flow of dilute polymeric solutions: Dynamical simulations and mechanism, D.G. Thomas, R. Sureshkumar and B. Khomami, *Phys. Rev. Lett.*, 97, 054501 (2006).
12. Least-square deconvolution: A framework for interpreting short tandem repeat mixtures, T.W. Wang, N. Xue and J. D. Birdwell, *J. Forensic Sci.*, 51,1284-1297 (2006).
13. An experimental study of slip flow in capillaries and semi-hyperbolically converging dies, P.A. Kamerkar and B.J. Edwards, *Polym. Eng. Sci.*, 47, 159-167 (2007).
14. Comparison of rheological properties of perfluoropolyethers through simulation and experiment, B. Jiang, N.J. Crawford, D.J. Keffer, B.J. Edwards, and J.J. Adcock, *Mol. Sim.*, 33, 881-888 (2007).
15. A molecular dynamics study of a nafion polyelectrolyte membrane and the aqueous phase structure for proton transport, S. Cui, J. Liu, M. Esai Selvan, D.J. Keffer, B.J. Edwards, and W.V. Steele, *J. Phys. Chem. B*, 111, 2208-2218 (2007).
16. A comparison between entropies of aromatic compounds from quantum mechanical calculations and experiment, M. Kassaee, W.V. Steele, and D.J. Keffer, *J. Molecular Structure: THEOCHEM*, 800, 23-34 (2007).
17. Measuring coexisting densities from a two-phase molecular dynamics simulation by Voronoi tessellations, J.T. Fern, D.J. Keffer and W.V. Steele, *J. Phys. Chem. B*, 111, 3469-3475 (2007).

New Grants, Contracts and Patents

For the period of July 1, 2006 to June 30, 2007.

1. Spinning of carbon fiber precursors from lignin, S. Petrovan, Oak Ridge National Laboratory, $32,281, 02/01/2007–06/30/2008.
2. Photosynthetic biohydrogen: An all-worlds solution to global energy production, P.D. Frymier and R.M. Counce, Environmental Protection Agency, $10,000, 10/1/2006–9/3020/07.
3. An investigation of anaerobic microbial fuel cell performance, P.D. Frymier, UTK-ORNL Joint Directed Research and Development Program, $49,061, 1/1/2007–12/31/2007.
4. Multi-scale modeling: application to hydrogen and helium in steels (renewal), D.J. Keffer, B.J. Edwards and D. Nicholson, The University of Tennessee Science Alliance JDRD Program, $52,200, 1/01/2007–12/31/2007.
5. Ash Pond Management in Coal-Fired Electricity Generation Facilities, R.M. Counce and P.R. Bienkowski, Electric Power Research Institute, $5,000, April 2007.
6. Development of Acetic Acid removal Technology for the UREX+ Process, R.M. Counce and J.S. Watson, U.S. Department of Energy (Nuclear Energy Research Initiative), $111,000, 5/15/2007–5/14/2008.
7. Ash Pond Modeling and Computer Simulation to Predict and Efficiently Control Ammonia/Nitrates and Heavy Metals at Discharge, R.M. Counce, P.R. Bienkowski and N. Handagama, Tennessee Water Resources Research Center, $25,000 per year, renewal, 6/1/2007–5/31/2008.
8. Interfacial dynamics in displacement flows of entangled polymeric fluids, B. Khomami, National Science Foundation, $200,000, 4/01/2007–3/31/2010.
9. Atomistic simulation of interfacial metal ion exchange, B. Khomami, University of Tennessee Science Alliance, $43,240, 1/01/2007–12/31/2007.
10. Processing of advanced nanostructured particles/films via aerosol routes, B. Khomami, Washington University--Center of Material Innovation, $15,000, 9/01/2006–8/31/2007.
11. Design of CVD reactors: A multiscale modeling approach, B. Khomami, MEMC Corporation, $30,000, 9/01/2006–8/31/2007.
12. Least-square deconvolution (LSD): A method to resolve DNA mixtures, T.W. Wang, N. Xue, J.D. Birdwell, M. Rader and J. Flaherty, U. S. Patent # 7,162,372 (2007).
13. Next generation CODIS, T.W. Wang and J.D. Birdwell, Unisys Corporation, $54,000, 3/1/2006–7/31/2006.
14. Next generation CODIS, Federal Bureau of Investigation, T.W. Wang and J.D. Birdwell, $830,000, 10/1/2006–9/30/2007.
15. Low cost carbon fiber technology development and concrete composite, S. Petrovan and D. Penumadu, University of Tennessee Space Institute, $89,542, 8/15/06–8/14/07.

Conferences and Invited Presentations*

For the period of July 1, 2006 to June 30, 2007.

1. A reagent-less enzymatic amperometric alcohol biosensor using the vertically aligned carbon nanofiber (VACNF), M.L. Weeks, T. Rahman, P.D. Frymier, S.K. Islam and T.E. McKnight, Nano and Giga Challenges in Electronics and Photonics, Phoenix, AZ, March 12-16, 2007.
2. Spinning carbon fiber precursors from 1-butyl-3-methylimidazolium chloride cellulose solutions, R. J. Sammons, J. R. Collier, S. Petrovan and B. J. Collier, The Fiber Society 2007 Spring Conference, Greenville, SC, May 23-25, 2007.
3. Elongational rheology and orientation number of polymer melts and solutions, J.R. Collier and S. Petrovan, The Fiber Society 2006 Fall Annual Meeting and Technical Conference, Knoxville, TN, Oct. 10-12, 2006.

4.* Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, B.J. Edwards, University of Alabama-Huntsville, Huntsville, AL, Sept. 22, 2006.

5.* Current research activities in microstructured materials of potential interest to Eastman Chemical, D.J. Keffer, B.J. Edwards and B. Khomami, Kingsport, TN, Jan. 30, 2007.

6.* Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, B.J. Edwards, University of Patras, Patras, Greece, June 21, 2007.

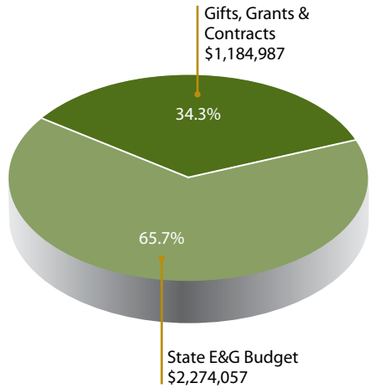
7. Correlation-based coarse-graining approach to coupling length scales: Atomistic to continuum, D.M. Nicholson, P. Nukala, Y. Osetsky, R. Stoller, C. Gao, D.J. Keffer and B.J. Edwards, NanoFocUL 2006 Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, August 24-25, 2006.
8. A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards and D.J. Keffer, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
9. A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the NVT, NpT and MuVT ensembles, J. Santiago, D.J. Keffer, B.J. Edwards and C. Baig, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
10. Flow of polymer blends between concentric cylinders, M. Dressler, B.J. Edwards and E.J. Windhab, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
11. A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards and D.J. Keffer, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
12. Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, T. Ionescu, B.J. Edwards, D.J. Keffer and V. Mavrantzas, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
13. Comparison of short and long chain polyethylene atomistic dynamics under shear and planar elongational flows, J.M. Kim, C. Baig, B.J. Edwards and D.J. Keffer, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
14. A generalized Hamiltonian-based algorithm for rigorous nonequilibrium molecular dynamics simulation in the NVT ensemble, J.G. Rajkumar, D.J. Keffer, B.J. Edwards and C. Baig, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
15. A comparison of rheological and structural properties of linear polyethylene melts under shear and elongational flow using nonequilibrium molecular dynamics simulations, J.M. Kim, C. Baig, D.J. Keffer and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
16. A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards and D.J. Keffer, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
17. Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer and V. Mavrantzas, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
18. A molecular dynamics study of nafion polyelectrolyte membrane and the aqueous phase structure for proton transport, S.T. Cui, J. Liu, M. Esai-Selvan, D.J. Keffer, B.J. Edwards and W.V. Steele, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
19. Estimation and analysis of the rheological properties of perfluoropolyethers, B. Jiang, D.J. Keffer and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
20. Understanding fuel cell operation through neutron imaging, D. Aaron, S. Yiacoumi, C. Tsouris, S.T. Cui, J. Liu, M. Esai Selvan, D.J. Keffer, B.J. Edwards and W.V. Steele, Imaging and Neutrons 2006 Workshop, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN, October 2006.

Conferences and Invited Presentations (con't.)

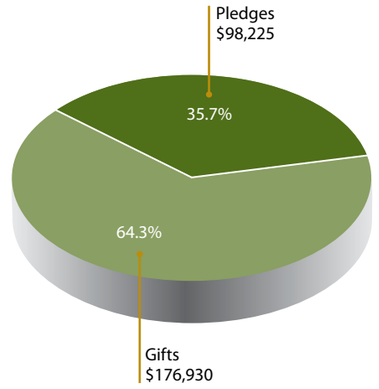
21. A molecular-level reaction algorithm for proton transport consistent with quantum mechanical transition state theory and macroscopic conductivity, by D.J. Keffer, M. Esai Selvan, J. Liu, S. Cui, B.J. Edwards and W.V. Steele, Electrochemical Society Annual Meeting, Chicago, IL, May 6-10, 2007.
22. Rheological and entanglement characteristics of linear chain polyethylene liquids in planar Couette and planar elongational flows, J.M. Kim, D.J. Keffer, M. Kröger and B.J. Edwards, XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007), Rhodes, Greece, June 6-10, 2007.
23. Absorbing boundary conditions for molecular dynamics and multiscale modeling, S. Namilae, D.M. Nicholson, P.K.V.V. Nukala, C.Y. Gao, Y.N. Osetsky and D.J. Keffer, The 2007 John H. Barrett Memorial Lectures: Multi-Scale Modeling and Simulation in Materials Science Workshop, The University of Tennessee, Knoxville, TN, April 2007.
24. Surfactant and electric field strength effects on surface tensions at liquid/liquid/solid interfaces, J. Santiago, D.J. Keffer and R.M. Counce, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
25. Computing thermophysical properties of aromatic compounds: Comparison of theory and experiment, M. Kassaee, D.J. Keffer and W.V. Steele, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
26. Using Voronoi tessellations to measure coexisting densities for molecular dynamics simulations, J.T. Fern, D.J. Keffer and W.V. Steele, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
27. Proton transport at the electrode/electrolyte interface of PEM fuel cells, D.J. Keffer, DOE Annual Contractors' Meeting, Washington DC, May 2007.
28. Primo Levi's 'The Periodic Table: The Chemistry of Literature', D.J. Keffer, Drew University, Madison, NJ, Sept. 2006.
29.* Computational and experimental study of high-performance lubricants in extreme environments, D.J. Keffer, AFOSR Tribology Program Review Meeting, Air Force Research Lab, Dayton, OH, Aug. 2006.
30. The molecular structure of hydrated nafion membrane interfaces: Developing a model for proton transport, D.J. Keffer, Nuclear Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, Aug. 2006.
31.* Dynamics of macromolecular solutions: Coarse graining, scission and confinement, B. Khomami, ICAM Workshop on Multiscale Interactions and Dynamics in Complex Biological Systems, St. Louis, MO, May 2006.
32.* Dynamics of dilute macromolecular solutions: Coarse graining strategies and multiscale flow simulation, B. Khomami, V. Venkataramani, A. Koppol and R. Sureshkumar, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 2006.
33.* Dynamics of dilute macromolecular solutions: Coarse graining, scission and confinement, B. Khomami, ORNL/CNMS NanoFocUL Workshop, Oak Ridge, TN, Aug. 2006.
34. Pattern formation in viscoelastic Taylor-Couette flow: Ribbons, oscillatory strips, disordered states and diwhirls, D.G. Thomas, R. Sureshkumar and B. Khomami, 78th Annual Meeting of the Society of Rheology, Portland, ME, Oct. 2006.
35. Hi-fidelity coarse grained models for dynamics of dilute polymeric solutions, V. Venkataramani, R. Sureshkumar and B. Khomami, 78th Annual Meeting of the Society of Rheology, Portland, ME, Oct. 2006.
36. Effect of counter-ion concentration on the rheology of shear-thickening surfactant solutions, M. Vasudevan, B. Khomami, A. Shen and R. Sureshkumar, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
37. Simulation of gas-liquid homogeneous nucleation: A molecular dynamics study, S. Dhumal, R. Lovett and B. Khomami, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
38. Spatio-temporal pattern formation in viscoelastic Taylor-Couette flow: Dynamical simulation and mechanism, D.G. Thomas, B. Khomami and R. Sureshkumar, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
39. Dynamics of polymeric solutions in prototypical processing geometries: A multiscale simulation approach, A.P. Koppol, R. Sureshkumar and B. Khomami, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
40. An efficient algorithm for multiscale flow simulation of dilute polymeric solutions using bead-spring chains, A.P. Koppol, R. Sureshkumar and B. Khomami, AIChE Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
41. Polymer induced drag reduction: The interplay between vortex dynamics and drag reduction, C.F. Li, R. Sureshkumar and B. Khomami, 59th Meeting of the American Physical Society, Tampa Bay, FL, Nov. 19-21, 2006.
42. Modeling the propagation of shear bands in metallic glasses, B.J. Edwards, B. Khomami and P.K. Liaw, 136th Annual Meeting of TMS, Orlando, FL, Feb. 25-Mar. 1, 2007.
43. Frictional drag properties of polymeric solutions in complex kinematics flows: A multiscale simulation approach, A.P. Koppol, R. Sureshkumar and B. Khomami, XVth International Workshop on Numerical Methods for Non-Newtonian Flows, Rhodes, Greece, June 6-10, 2007.
44.* Solution to the missing person identification: Theory and implementation, T.W. Wang, FBI Workshop for CODIS End Users, Reston, VA, April 2007.

Financial Information

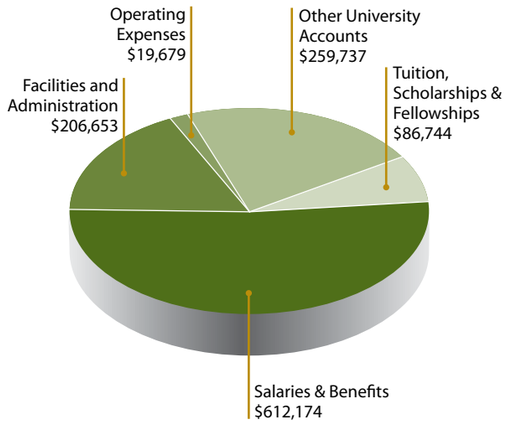
Total Income/Revenue for FY 2007—$3.46 Million



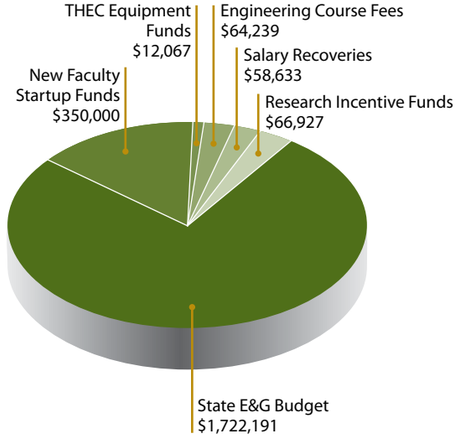
Gifts and Pledges for FY 2007—$275,155



Gifts, Grants and Contract Expenditures for FY 2007—$1.19 Million



Educational and General Income/Revenue for FY 2007—$2.27 Million



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