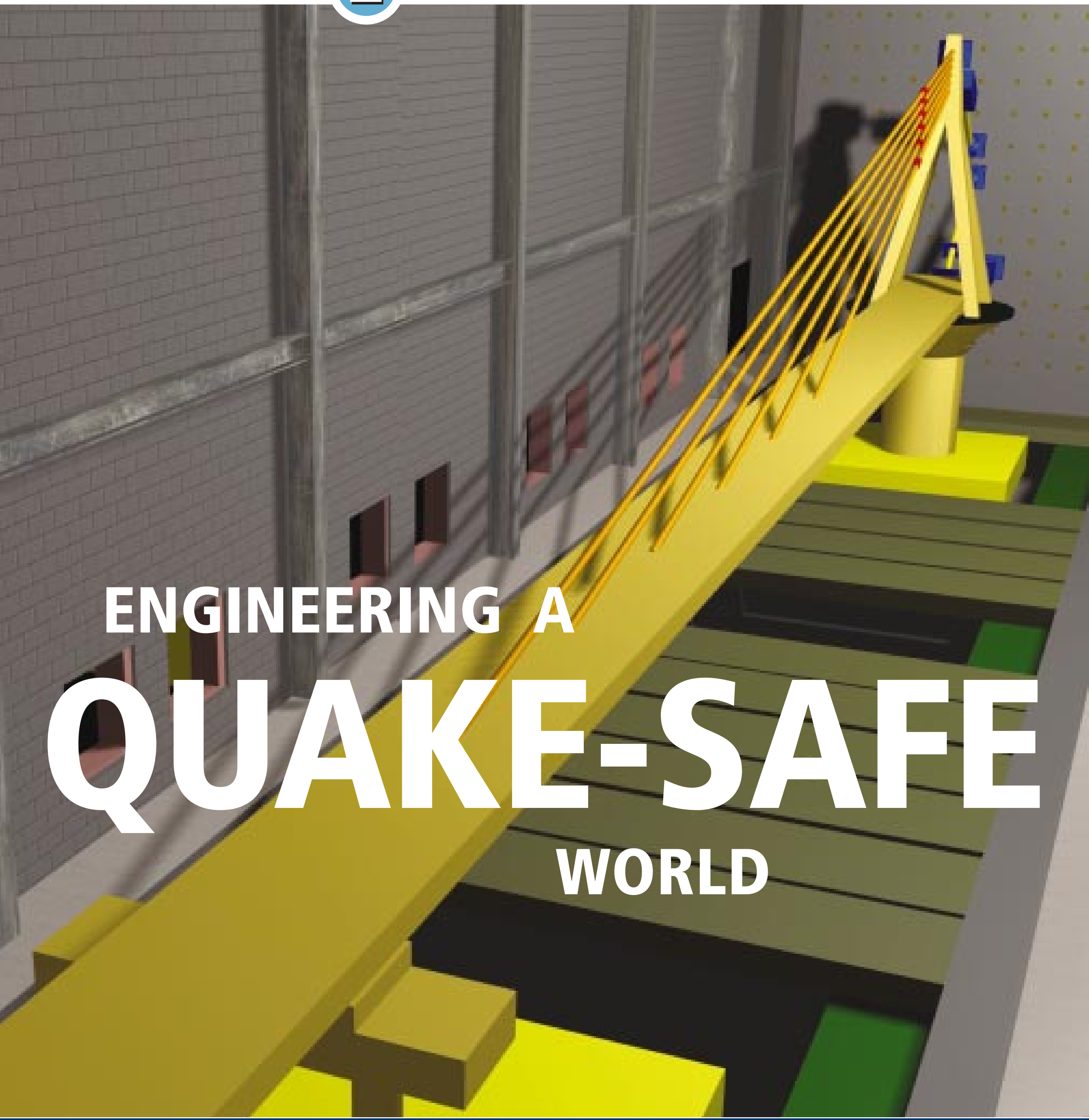


ENGINEERING A QUAKE-SAFE WORLD

School of Engineering and Applied Sciences
University at Buffalo The State University of New York
www.eng.buffalo.edu

JUNE 2003

Mark H. Karwan
Professor and Dean

I am pleased to share with you our second publication in a six-issue series explaining our school's research focus areas as they relate to our strategic objective to "perform high quality research that advances applied science or technology while preparing future researchers for industrial, academic and government positions."

In this issue, we focus on infrastructure and environment. Major areas addressed by our faculty include the design and retrofit of systems using earthquake and multi-hazard resistance technologies; the design and sustainability or the correction of environmental systems using biological, chemical and/or physical means as well as algorithmic solutions; and the development of new materials. As in the first issue, we've also included a recent major award and a recognition won by our faculty.

The work described herein is providing scientific and engineering leadership to the shaping of today's and tomorrow's infrastructure and environment. Please enjoy our faculty and school accomplishments.

Igniting Ideas Series available at: www.eng.buffalo.edu/IgnitingIdeas

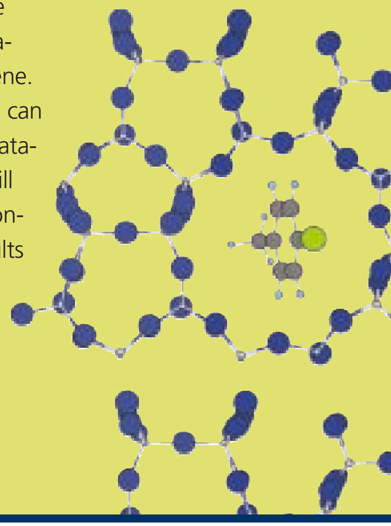
Produced by the University at Buffalo Office of Creative Services, University Communications. June 2003. C 10328-03.

The Greening of Aromatic Chlorination Processes

Many plastics, specialty polymers, pharmaceuticals, dyes, fragrances and pesticides use chlorinated aromatics as intermediates. The processes for producing the chlorinated aromatics generate undesired chlorinated aromatic byproducts.

The strategy of Carl Lund, professor and chair of chemical engineering, and his research group is to make the chlorination process "greener" by developing heterogeneous catalysts to replace soluble acids. Such catalysts can be separated from the products without the use of water, eliminating the aqueous waste stream. The challenge lies in also eliminating the undesired chlorinated aromatic products. The research group is using a combination of experimental testing and computational chemistry to find materials that are more selective and thereby produce more para-chlorotoluene and less ortho-chlorotoluene.

The group has found that L zeolites can be selective when used as chlorination catalysts, but the lifetime of the zeolites is still too short. Thus experimental research continues, building upon the promising results to date. The goal is to design polymer-based catalyst materials and templated inorganic materials with the same selectivity as the L zeolites, but sustain their catalytic activity indefinitely.



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UB'S MCEER AND THE FUTURE OF seismic science

UB's Multidisciplinary Center for Earthquake Engineering Research (MCEER), established in 1997, builds upon the previous National Center for Earthquake Engineering Research at UB, which was founded by the National Science Foundation in 1986. MCEER seeks solutions to reduce earthquake losses and help communities stand better prepared and increasingly resilient when faced with earthquakes. Projects focus on technologies to strengthen critical facilities that communities depend upon in times of crisis (e.g., hospitals, highways, and utilities), and to improve post-earthquake emergency response, crisis management, and recovery.

MCEER believes that the future of earthquake engineering lies in advanced and emerging technologies that include:

- Site remediation technologies—to improve and stabilize soils and foundations
- Structural control and simulation—to protect structures from damaging vibrations
- High-performance materials—to strengthen buildings, bridges, soils and pipelines
- Condition assessment technologies—to better estimate potential and actual earthquake losses

PHOTO: DR. MICHAEL CONSTANTINOU

- Decision support systems—to enhance emergency response and post-earthquake recovery

MCEER is currently exploring these crucial technologies within four research programs: Seismic Evaluation and Retrofit of Lifeline Networks; Seismic Retrofit of Hospitals; Emergency Response and Recovery; and Improving Seismic Performance and Reliability of the Nation's Highway System.

A fifth thrust—Facilities and Computational Networks in Earthquake Engineering—seeks to network many of the nation's premier computational and experimental facilities for advanced analytical, geotechnical, and structural earthquake engineering studies.

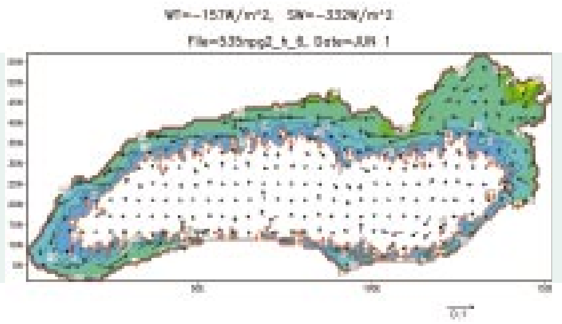
MCEER forges strategic alliances with manufacturers, consultants, end-users and other public- and private-sector stakeholders to develop, adapt, test, and help implement use of new and emerging technologies to mitigate earthquake losses. It also provides partner access to research, education and technology transfer opportunities including state-of-the-art knowledge, experimental facilities, information resources, publications, seminars, short courses, and distance learning.

MCEER contributions to advancements in seismic isolation and damper technologies, and developments in computer modeling and simulation, have helped pave the way for increased application of a variety of protective systems in new construction and retrofit of buildings, bridges, and lifelines around the world.

George C. Lee, Samuel P. Capen Professor of Engineering, and Michel Bruneau, professor of civil, structural and environmental engineering, are supported and advised by senior staff and committees regarding center research, administration, and outreach initiatives.

Great Lakes Program Activities—Lake Ontario

The UB Great Lakes Program (GLP) has simulated Lake Ontario over the past decade, which has led to a state-of-the-art water quality model–the Lake Ontario Toxics Model, version 2 (LOTOX2)–developed by Joseph DePinto, civil, structural and environmental engineering (CSEE) research professor with researchers at UB, Clarkson University, the National Water Research Institute in Canada, and the New York Great Lakes Research Consortium at SUNY College of Environmental Science and Forestry (ESF). Funding originated from the consortium and continued from the U.S. Environmental Protection Agency (EPA). Currently, two projects are seeking to improve model performance by linking it with a hydrodynamic model to provide mixing and circulation information for transport calculations, and to extend the modeling capabilities by incorporating a sub-model to simulate mercury transport and transformations. Joseph Atkinson, GLP director and CSEE professor, James Jensen, CSEE associate professor and DePinto are heading these efforts with New York State Department of Environmental Conservation and EPA staff. The model estimates total maximum daily load for contaminants. The sub-model will evaluate the dangers that concentrations pose for human and ecosystem health.



Related modeling of Lake Ontario involves detailed hydrodynamic and temperature models. An Atkinson master's student recently completed a comprehensive numerical model that evaluates the lake's thermal cycle. It is being extended to provide fast response predictions of algal bloom transport in Lakes Ontario and Erie. The project, with Atkinson as PI, is part of a five-year study headed by Gregory Boyer at SUNY ESF, funded by the National Oceanic and Atmospheric Administration. This first harmful algal bloom study conducted in fresh waters represents a new direction in Great Lakes research.

Atkinson is also the U.S. lead for the Environmental Technical Working Group's five-year International Joint Commission study to evaluate the water level regulation plans for outflows of Lake Ontario into the St. Lawrence River.

ENGINEERING AT THE EDGE

Debris flows and virtual volcanoes

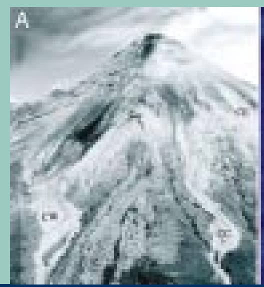
Technologies ranging from mathematical modeling, geologic simulation and geographic information science to scientific computing and virtual reality are being combined to provide accurate information on the geologic dangers of volcanoes.

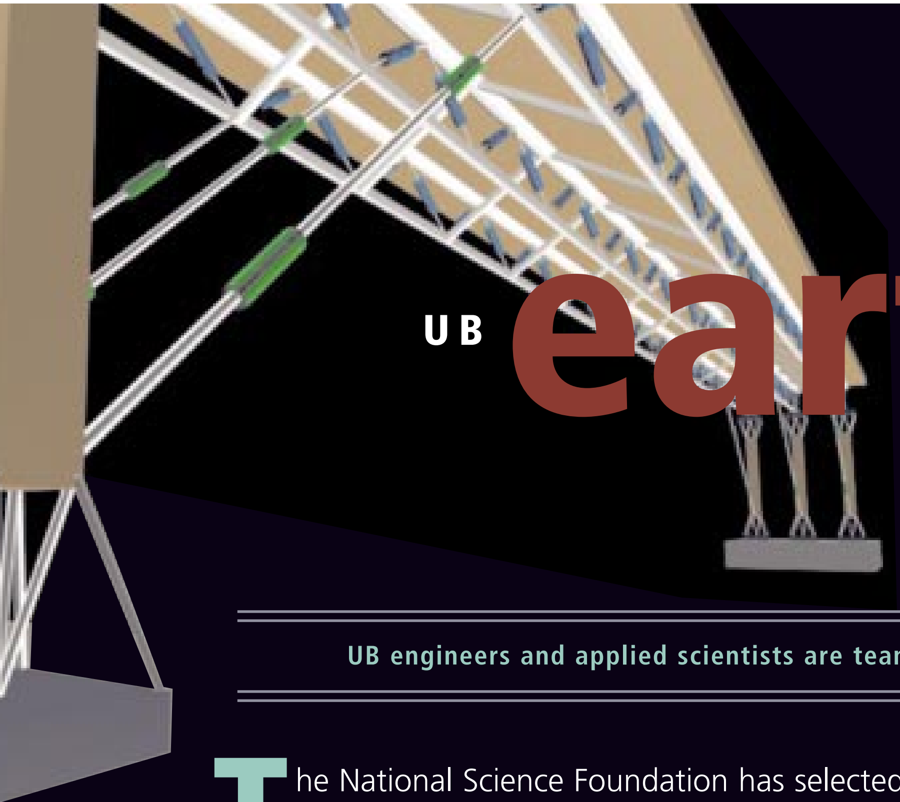
Coordinating with counterparts in Mexico and focusing on three volcanoes in that country, researchers at the University at Buffalo are simulating rock avalanches and pyroclastic and debris flows. The UB research team led by Abani Patra, associate professor of mechanical and aerospace engineering and principal investigator, is using novel computational methods to work on large-scale numerical computations whose outputs are very large data sets that must be converted into suitable visual formats for users ranging from scientists to public-safety planners. The simulations consider many complex variables including the rough terrain and physics at multiple scales.

Patra is joined by Michael Sheridan and Marcus Bursik from geology, E. Bruce Pitman from mathematics, Christina Bloebaum, Thenkurussi ("Kesh") Kesavadas and Eliot Winer from mechanical and aerospace engineering and C. Renschler from geography. They are using satellite data from volcanoes to develop realistic models and simulations of geophysical mass flows.

The end product will integrate simulation results, remote sensing data and geographic information system data to present the information for scientists, decision-makers and, ultimately, citizens. The work is being conducted under a grant from the National Science Foundation's Information Technology Research Program.

Simulation of flows at Volcan de Colima by B. Rupp and M. Bursik using the newly developed TITAN2D code





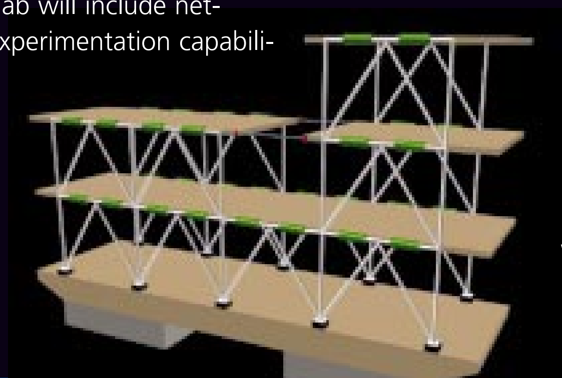
UB earthquake RESEARCH GETS A MULTIMILLION DOLLAR UPGRADE

UB engineers and applied scientists are teaming up to help ensure that our buildings and bridges stand the tests of time

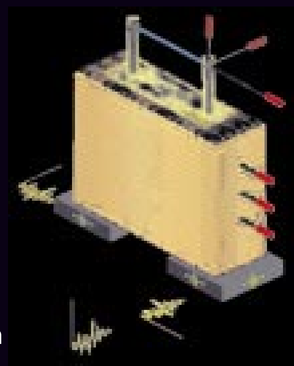
The National Science Foundation has selected UB's Structural Engineering and Earthquake Simulation Laboratory (SEESL) to become a key node in the George E. Brown, Jr. Network for Earthquake Engineering Simulation (NEES) nationwide earthquake engineering collaboratory.

Under NEES, the SEESL facility is receiving $20 million in upgrades: dual, movable, six-degrees-of-freedom shake tables capable of subjecting specimens weighing up to 100 metric tons and measuring up to 120 feet to fully in-phase or totally uncorrelated dynamic excitations, a large reaction wall, a significantly expanded strong floor area, high-performance dynamic and static actuators, and associated hydraulic and control systems. The upgraded facility will be capable of testing full or large-scale structures using static or dynamic loading. Along with conventional static, quasi-static, and dynamic force techniques, modern techniques such as pseudo-dynamic, effective force, and real-time dynamic/pseudo-dynamic hybrid testing will be possible. In addition, a new form of testing—real-time dynamic hybrid testing—is being explored in which shake table/dynamic force experiments on substructures are combined in real-time with computer simulations of the remainder of the structure to provide a more complete picture of how earthquakes would affect large structures without physically testing the entire structure.

The new lab will include networked tele-experimentation capabilities tied to the testing systems using discrete and global sensors,



including high-resolution digital video and imaging capabilities.



After construction is completed, SEESL, which is also a principal facility for the Multidisciplinary Center for Earthquake Engineering Research (MCEER), will be among the most sophisticated structural testing facilities in the world.

The NEES project PI is Michel Bruneau; co-PI's are Andrei Reinhorn, Michael Constantinou, S. Thevanayagam, and Andrew Whittaker.

Going Public with New York State Brownfield Data

While extensive information on remediated properties is in the public domain, it can be very hard to access. To address this difficulty, a web accessible database is in its final stage of development with funding from the New York State Department of Environmental Conservation. A. Scott Weber, director of UB's Center for Integrated Waste Management and professor of civil, structural, and environmental engineering, heads a team with co-PI Douglas Flewelling from the National Center for Geographic Information Analysis and professor of geography.

Data are being formed from such cleanup programs as the NYS Superfund and the NYS Voluntary Cleanup programs. Site information includes location, history, contact information for involved persons, contaminants and their concentrations, remediation goals/standards, remedy if chosen, whether institutional and/or engineering controls have been implemented, and current use of the property. Users are able to query data via the web and represent these data visually through a graphical information system interface.

Examples of how the database will be used include access to information for transferability to future sites, knowledge of which remedies have been applied for specific contaminants, contact persons associated with those remedies, evaluating the background levels for contaminants throughout New York State, information on contaminant cleanup goals, the effectiveness of engineering controls, and evaluating how many sites have been made productive.

"This database and its accessibility is something the public is very excited about," says Weber. "In conversation after conversation there has been one consistent theme—'we need it now and we need it fast.'" Ultimately, the database will serve as a powerful tool for further UB research on how to remediate contaminated sites into productive ones.

Smart Design: Multifunctional Cement-Based Materials

Deborah D.L. Chung, Niagara Mohawk Chair Professor of Materials Research, and her research team explore multifunctional structural materials for infrastructure. Their goal is a structural material to serve one or more non-structural functions while retaining good structural properties.

A particularly valuable function is sensing. A self-sensing structural material allows the structure to "feel" what is going on, allowing the structure to be programmed to respond to the situation in an appropriate fashion. A structure that has such capabilities is said to be smart. Sensing is the most basic function of a smart structure.

The self-sensing of strain (i.e., deformation) is a function that is useful for vibration sensing and control, traffic monitoring, weighing, room occupancy monitoring, intruder detection, building security and facility management. In particular, room occupancy monitoring allows building energy savings through automatic control of the lighting, ventilation, air conditioning and heating in accordance with the number of people in each room. Additional benefits of such a material would include reduced cost, enhanced durability and repairability, increased functional volume, avoided degradation of the mechanical properties, and simplified design.

The research, which has been partially funded by the National Science Foundation, continues to be very fruitful. The functions attained in multifunctional cement-matrix composites include the self-sensing of strain, damage and temperature, self-heating and electromagnetic interference (EMI) shielding. The research program has resulted in approximately 100 journal publications since 1993; a book entitled Multifunctional Cement-Based Materials, Marcel-Dekker, in press; an issued patent; and world-wide press coverage.

Impacting Structures Across the Country and Around the World

UB professors are stimulating the advancement of structural engineering on a truly global scale. They helped develop advanced "toggle-brace" technology used in three 38-story buildings in Boston and San Francisco. Farther from home, professors provided engineering design to the Ataturk International Airport and the Bolu Viaduct in Turkey, the Sakhalin Gas Platforms in Russia and to LNG tanks in Greece. They investigated damage to structures and response of medical and emergency operations following the September 11 attacks on the World Trade Center. Their studies led to reports and a New York City workshop to examine and improve upon engineering and emergency response challenges posed by the disaster. UB investigators played lead roles in drafting building codes and guidelines for seismic safety.

They have also helped the local economy by broadening the product base of Western New York businesses: They helped Taylor Devices modify military damper technologies for seismic protection of buildings and other structures; they pioneered a "smart" earthquake-protection system that is being further developed by Enidine for earthquake protection and naval applications through a contract from the Defense Advanced Research Projects Agency; and they collaborated with Taylor Devices and Moog to develop active fluid dampers to reduce earthquake vibrations in structures by combining technologies originally developed for the B-2 Stealth Bomber.

Researchers at UB and a few other universities developed a first-ever computer program (IDARC) for damage analysis of concrete structures. The program enables engineers to analyze brittle concrete buildings and bridges to predict damage. A series of computer programs (3-D BASIS) was developed by UB and colleague researchers to enable practicing engineers to analyze the effectiveness of seismic isolation systems in complex structures—and have advanced the application of base isolation in the U.S. and abroad.

Global E³

D. Joseph Mook, professor of mechanical and aerospace engineering and assistant dean for international education, has been elected chair of the Global Engineering Education Exchange. Administered by the Institute of International Education, the Global E³ provides opportunities for students to receive academic credit for courses taken at overseas institutions and practical training in a foreign setting.

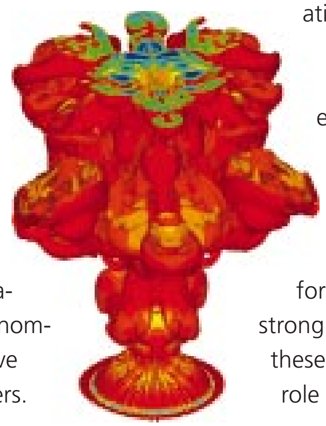
Under Mook's leadership, UB's engineering students more than double the national average at a five percent participation rate in study abroad programs.

An emerging leader

Jeffrey Errington, assistant professor of chemical engineering, is a 2003 National Science Foundation Career award winner. The designation recognizes and supports the early career-development activities of teacher-scholars who are most likely to become the academic leaders of the twenty-first century. A doctoral graduate of Cornell University, Errington's research interests include statistical thermodynamics, biopreservation, molecular simulation and the structure of complex fluids.

Using Chemistry and Computers to Study Fire Plumes

While Paul DesJardin, assistant professor of mechanical and aerospace engineering, is not playing with fire, he is researching the dynamics of large-scale fire plumes as they relate to the environment. His work is in high fidelity numerical simulations of fire phenomena using massive parallel computers.



He and his team are currently exploring the dynamics of large-scale fire plumes to better understand the soot and smoke generation processes that pollute our air and can have a devastating effect on our environment.

One finding concerns the role of turbulence-chemistry-radiation interactions on the soot-formation processes. The strong nonlinear coupling of these processes has a dominant role on how much and where the soot is formed in a fire. The interactions define the regions of hot soot—unburnt hydrocarbons—that radiate profusely. Thermal radiation from fires does adverse things like melting steel structures, and when steel structures melt, they break. Understanding turbulence-chemistry interactions can help prevent structural collapse during fire.

An aspect of this collaborative research with Sandia National Laboratory—numerical simulations of wall fires—is funded by the Office of Naval Research.

Routing of Hazardous Materials

The volume of hazardous materials—250,000 shipments daily in the U.S.—and the accompanying risk to citizens necessitates the development of guidelines to regulate their transport. And this is just what Rajan Batta and Mark Karwan, professors of industrial engineering and chair of the department and dean of the school, respectively, are doing—protecting the environment via operations research by finding the safest way to transport hazardous waste.

They develop and analyze quantitative models to assist creating rules of transport. Their models have evolved to include risk for a traveling vehicle, the equitable distribution of risk among communities, and a GIS-software that incorporates practical issues like changing accident probabilities and population shifts with the time of day. The hazardous materials modeled have various levels of toxicity—from routine materials like gasoline to extremely dangerous materials like spent nuclear fuel.

The program is supported by the National Center for Geographic Information Analysis—Buffalo, one of three sites designated and funded by the National Science Foundation. The work has produced several master's and doctoral students and resulted in numerous articles in such journals as Computers & Operations Research, European Journal of Operational Research, Information Systems and Operational Research, Operations Research, Operations Research Letters, Transportation Research and Transportation Science.

Sustainable Materials

Li Lin, professor of industrial engineering, is leading a team researching material selection in manufactured items by using green design and environmental cost analysis criteria. Joining Lin as principals are John Van Benschoten, civil, structural and environmental engineering and John Vena, social and preventive medicine. The three-year project is funded by EPA's STAR research program through a joint relationship between the NSF and the EPA called Technology for the Sustainable Environment.

The project builds on previous research by Lin and Alejandro Rivera, in which environmentally conscious criteria for products were developed and preliminary studies were conducted on the impact of product design decisions on human health. The current project looks at several critical issues: material selection at the design stage and its potential impact to human toxicity and eco-toxicity; environmental, economic, and social impacts of product design decisions; and environmental accounting models for sustainability management. The Xerox Corporation is providing engineering support and product samples.

Groundwater and the Great Lakes

When engineers conduct research on groundwater, they usually think of "large-scale" as one watershed—an area where all of the water on or under it drains into the same place, such as a lake and its tributaries. Using the three-hundred-node Dell high-performance computing cluster in UB's Center for Computational Research (CCR), Alan Rabideau and Igor Jankovic, associate professor and assistant professor respectively of civil, structural and environmental engineering, are working to turn that definition on its head.

The exchange between groundwater and the Great Lakes is not well understood, but is becoming increasingly important as cities that border the lakes, like Chicago, increase their reliance on groundwater.

The goal is to create what could be the first groundwater model capable of accurately representing how contaminants migrate through groundwater in multiple watersheds at a variety of scales, ranging from the size of individual grains of soil to bodies of water that cover many miles. Ultimately, they are interested in problems like climate change and its impact on the Great Lakes.

Jankovic uses the computer to describe the microscopic movement of contaminants that then helps identify the parameters for the equations in the model. At the same time, Rabideau studies the chemical-end of things, examining and accounting for how differences in individual soil particles influence contaminant transport in groundwater.

The research was initiated by an Environmental Protection Agency grant awarded to Rabideau in 2000. Since then, the National Science Foundation has awarded the team additional grants.