

ICTAS

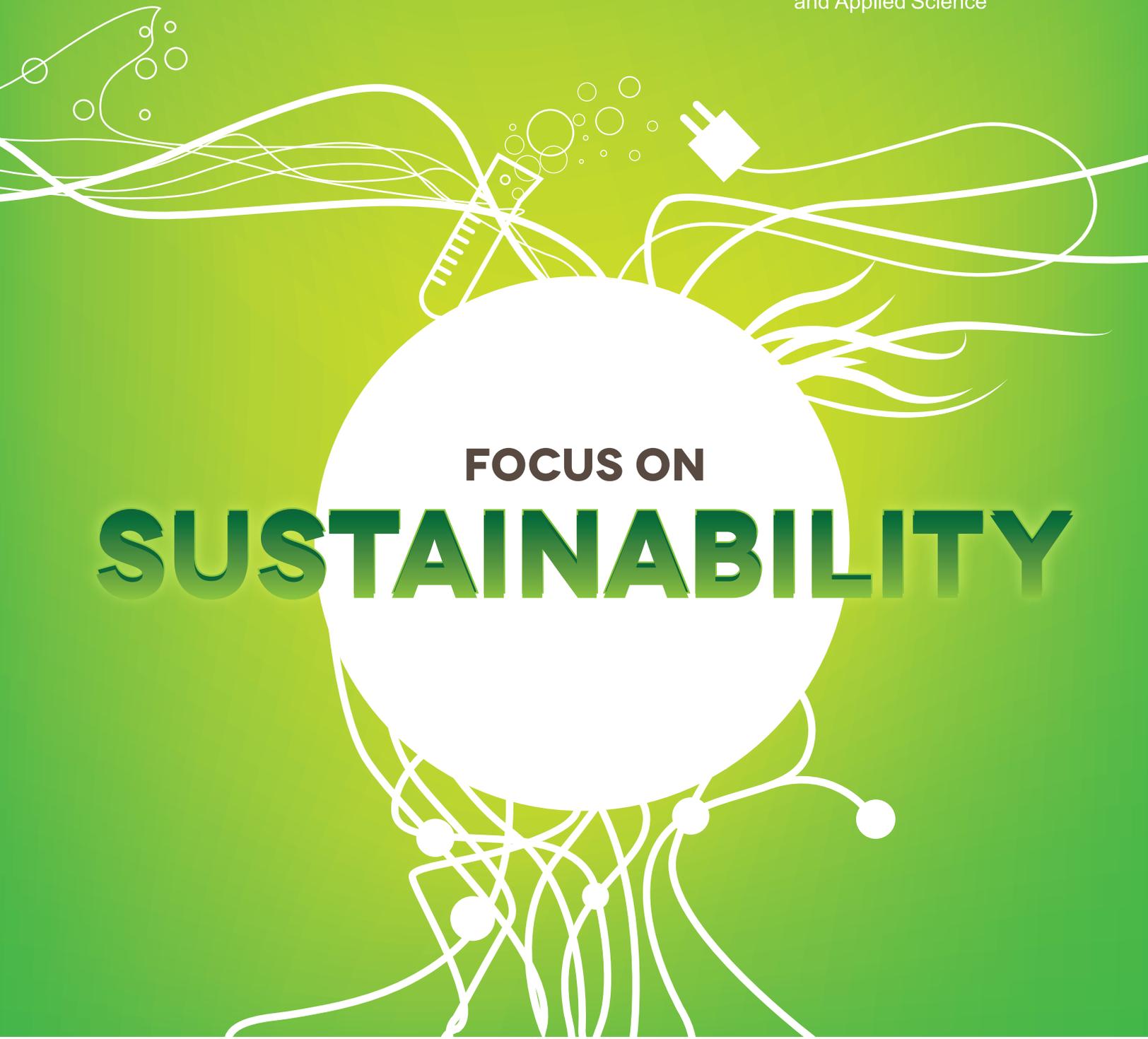
CONNECTION

ISSUE 12 • JANUARY 2013



VirginiaTech

Institute for Critical Technology
and Applied Science



FOCUS ON

SUSTAINABILITY

www.ictas.vt.edu • www.facebook.com/ictasvt

A VIRGINIA TECH RESEARCH INSTITUTE

:IN THIS ISSUE



SUSTAINABILITY and the FABRIC OF ICTAS RESEARCH

Building a future that includes the availability of water, energy, and other critical resources is a continuing concern for the world at large. ICTAS seeks to be a voice that provides solutions to this imminent concern.

- 03** Virginia Tech Receives Prestigious Sloan Foundation Grant to Examine the Building Plumbing Microbiome
- 04** New Faces at ICTAS
- 05** ICTAS Center of Excellence in Sustainable Water Infrastructure Management (ICE-SWIM) Launches WATERiD with New Grant
- 06** Water for Health
- 07** 2012 Doctoral Scholars
- 09** Virginia Tech's StREAM Lab: A "Common" for Interdisciplinary Research, Education, and Outreach Related to the Dynamics of Water and Societal Systems
- 10** Switchgrass Molecular Breeding Program Seeks to Reduce Oil Dependence
- 11** Using Emerging Engineering Technology to Enable Sustainable Agriculture
- 13** Sustainable Nanoenabled Consumer Products
- 15** Translational Nanomedicine for Healthy Citizens and a Sustainable Future
- 17** Advancing Coal and Biomass Gasification through Modeling
- 22** Blending Fuels for Improved Power Production



06



11

DIRECTOR'S CORNER

ROOP MAHAJAN • ICTAS DIRECTOR
(540)231-1929 • rmahajan@vt.edu



Sustainability and the Fabric of ICTAS Research

Sustainability, the overarching theme of this issue of the *ICTAS Connection*, is at the heart of the ICTAS vision which calls for ICTAS to be a premier institute that advances transformative, interdisciplinary research for a sustainable future. This vision reflects our firmly held view that food, water, energy, shelter, transportation, healthcare, and employment are the basic requirements for life and prosperity that should be met for every human. The big challenge is to uphold this lofty view without compromising the ability of future generations to meet their needs. This challenge recognizes that the environment--a provider of natural resources such as water, air, and sunlight that every living inhabitant of earth is dependent upon--is limited in its carrying capacity. Two major requirements, therefore, are that any development of the environment must be economically and socially sustainable.

To realize these two requirements, ICTAS research strategy calls for harnessing and leveraging the collective talents of Virginia Tech faculty and researchers in a few of the most powerful converging technologies of the 21st century--nanotechnology, information technology, cognitive science, and modern biology. Guided by the principles of sustainability, we have organized these technologies around the following research thrusts: (i) Nanoscale Science and Engineering, (ii) Nano-Bio Interface, (iii) Sustainable Energy, (iv) Renewable Materials, (v) Sustainable Water, (vi) Cognition and Communication, and (vii) Homeland Security. These thrusts are supplemented by an Emerging Technologies research thrust that is designed to promote blue-sky thinking and to identify the disruptive technologies of the future. ICTAS makes investments in these strategic research thrusts by providing infrastructure and financial support for seed research projects selected through an annual peer-reviewed process. Successful projects are thematically brought together to establish ICTAS centers that are targeted for additional investment so that they can achieve growth and national recognition. The scholarship and research expenditure goals for these centers mirror the institute's overall goals.

Our efforts to create a sustainable future face a daunting set of complex, challenging, and interconnected problems affecting water, energy, the environment, health, poverty, terrorism, and war, to name a few. Resolving these problems will require a healthy dose of innovation, multiple perspectives, teamwork, and a culture of nimbleness that enables us to change course midstream if needed.

Interdisciplinary research as a mode of discovery and learning is a powerful paradigm for meeting the challenges confronting sustainability. It allows us to break down and restructure our knowledge about this subject so that we gain new insights and use our imaginations to invent and innovate. The report *Facilitating Interdisciplinary Research* from the National Academies Press, 2005, considers interdisciplinary research to be "one of the most productive and inspiring of human pursuits--one that provides a format for conversations and connections that lead to new knowledge."

The projects described in the following pages exemplify how our researchers push the envelope of science and technology with sustainability woven into the fabric of their research. I hope that you will enjoy this issue of the *ICTAS Connection* and that you will join us in our efforts to apply and develop technologies and practices that will create a sustainable future.



AMY PRUDEN • ASSOCIATE PROFESSOR,
CIVIL & ENVIRONMENTAL ENGINEERING
(540)231-3980 • apruden@vt.edu

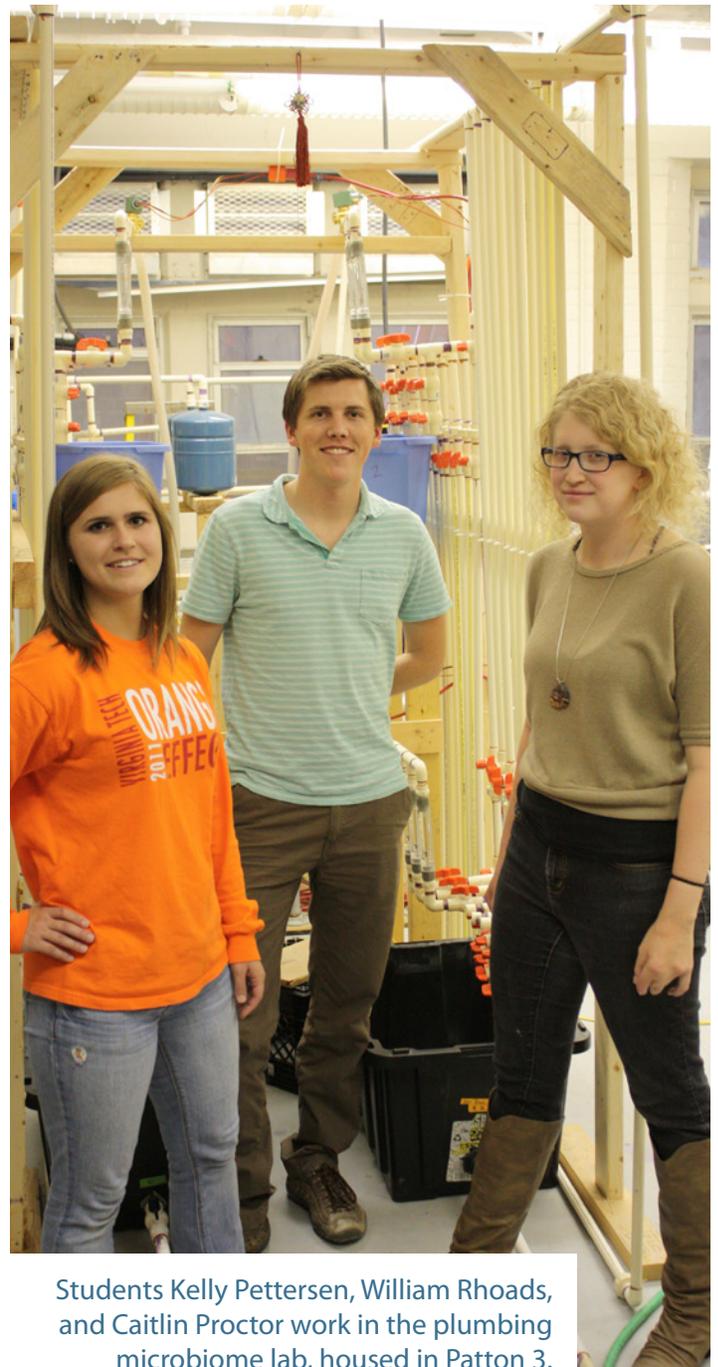


Virginia Tech Receives Prestigious Sloan Foundation Grant to Examine the Building Plumbing Microbiome

The Alfred P. Sloan Foundation announces funding for a new study examining the effect of pipe materials, water flow, and chemistry on the types of microorganisms found in building plumbing systems and considers health implications for building occupants. This work will be performed by ICTAS Water Group members Drs. Amy Pruden and Marc Edwards (Civil and Environmental Engineering) and by Dr. Annie Pearce (Department of Building Construction) at Virginia Tech and by Dr. Anisha Patel (School of Medicine) at the University of California San Francisco. The interdisciplinary research will have a special emphasis on problems commonly encountered in schools and new green buildings, where water tends to sit in plumbing for long time periods before it is used.



Building plumbing systems deliver fresh potable water for drinking and bathing to consumers, and this water sometimes contains harmful microorganisms that can cause consumers to become sick. Researchers are especially concerned about harmful microorganisms that can grow rapidly in hot water tanks and building plumbing and that are known to cause Legionnaires' disease and other health problems. The new research will use field and laboratory test rigs to examine simple approaches that can stop the growth of these harmful microorganisms, including disinfectants and high temperatures. Next-generation DNA sequencing technology will be used for the first time to probe the full depth of bacteria, protozoans, and viruses that inhabit building plumbing systems. Principal investigator Dr. Amy Pruden-Bagchi stated: "It is our hope that understanding the plumbing microbiome will open new doors to advancing the health of our water, in the same way that modern medicine is now being enhanced by discovery of the microbiome of the human body."



Students Kelly Pettersen, William Rhoads, and Caitlin Proctor work in the plumbing microbiome lab, housed in Patton 3.

New Faces at ICTAS



Ronaka Adams, Receptionist, ICTAS I

Ronaka has an associate degree in computer-aided drafting and is currently pursuing her B.S. in sociology. She joined ICTAS after having been employed as a preschool teacher and a 911 dispatcher. In her free time, Ronaka enjoys painting acrylics on mixed media, and crafting wooden signs and monograms. She lives in Radford with her husband, John.



David Ashwell, Desktop Support Tech, IT

David graduated from Virginia Tech last December after completing a degree in agriculture and applied economics. He hopes to pursue a bachelor's degree in mechanical engineering in the coming years as a part-time student. David has worked in IT-related fields for just over 4 years. His interests include computers, gaming, sports, outdoor activities, and spending time with his girlfriend, Lessa.



Rachel Born, Student Assistant

Rachael Born is interested in sustainability and energy systems, and her self-designed B.S. in environmental physics from the College of William and Mary reflects that interest. Currently, she takes undergraduate courses in electrical engineering with the goal of earning a master's degree. Rachel's hobbies include traveling wherever she can, hiking around the Blue Ridge, and reading thick books. At ICTAS, she supports research program managers Mr. Jeff Beeby and Dr. Matt Hull.



Jennifer Cacciola, Administrative Assistant, Research

Jennifer has a bachelor's degree in biology from Virginia Tech. She is happy to have rejoined the Virginia Tech family having previously been employed as a laboratory and research specialist with the Virginia-Maryland Regional College of Veterinary Medicine and as a research technician for a private industry research and development laboratory located in the Corporate Research Center. In her free time, Jennifer enjoys running, hiking, playing volleyball, photography, and cheering on the Hokies. Jennifer lives in Christiansburg with her husband, Steve.



John Di Stefano, Student Assistant, Facilities

A sophomore in biological sciences at Virginia Tech, John was born and raised in Virginia. He has always loved the outdoors and is especially fond of the different geographical regions of his home state. John's family consists of a brother, two sisters, and his parents who have been married for almost 30 years. John is also a proud uncle of two nieces.



Kelsey Klarman, Student Assistant, Research

A Virginia Tech student, Kelsey is studying construction engineering and management and plans to graduate with the class of 2015. Kelsey is also pursuing a minor in green engineering. When school work is out of the way, she enjoys participating in Habitat for Humanity builds, staying involved in the Virginia Tech community, and watching the Baltimore Ravens, her hometown team, play football.



Ryan Oberholzer, Student Assistant, Communications

Ryan, a sophomore at Virginia Tech, is originally from Woodstock, Maryland. His current major is mechanical engineering. Ryan hopes to graduate from Tech, secure employment at an engineering firm, and possibly attend graduate school. In his free time, Ryan is a mentor in Virginia Tech's Galileo Engineering Learning Community for Men where he creates and organizes service events.



Lisa Stables, Fiscal Team Manager

Lisa joined ICTAS in September 2012. As fiscal team manager, she is responsible for financial and human resource management. Lisa has 25 years' experience, including 15 years at Virginia Tech working in administrative, human resource, and financial administration positions. Prior to joining ICTAS, Lisa served as business manager for Virginia Tech's physics and mechanical engineering departments and for the Virginia Tech Foundation.



Christopher Winkler, Senior Research Associate

Chris earned his bachelor's from Rice University and his Ph.D. from Drexel University. Our newest employee, Chris was hired to help operate and maintain the electron microscopy equipment located in the ICTAS Nanoscale Characterization and Fabrication Laboratory. Experienced with a range of scanning and transmission electron microscopy techniques and sample preparation, Chris specializes in the development of preparation procedures that enable the in situ characterization of materials inside the electron microscope.

SUNIL SINHA • ASSOCIATE PROFESSOR,
CIVIL & ENVIRONMENTAL ENGINEERING
(540)231-9420 • ssinha@vt.edu



ICTAS Center of Excellence in Sustainable Water Infrastructure Management (ICE-SWIM) Launches WATERiD with New Grant

Problems with old, leaking, and bursting water pipes are expected to cost over 1 trillion dollars in the next 30 years and will result in the loss of about 10-15% of treated potable water before it even reaches homes and buildings. A new grant from The Water Environment Research Foundation (WERF), via a cooperative agreement with the U.S. Environmental Protection Agency (EPA), has created WATERiD, an on-line living knowledge base that permits utilities to easily improve how they manage, upgrade, and restore this critical infrastructure. Developed by Dr. Sunil Sinha, associate professor of civil and environmental engineering at Virginia Tech, and co-director of ICE-SWIM, WATERiD is unique in that it allows utilities to efficiently share their “lessons learned” from hard experiences. Other participating utilities can access this information via the Internet. “Having an expansive knowledge base for condition assessment and renewal technologies that can assist drinking water and wastewater entities to more effectively put comprehensive asset management into practice, and meet their Clean Water Act and Safe Drinking Water Act requirements, fits well with the EPA’s long-standing research investment into managing our nation’s water infrastructure,” stated Thomas F. Speth, Ph.D., P.E., Director, Water Supply & Water Resources Division, National Risk Management Research Laboratory, U.S. EPA Office of Research and Development.

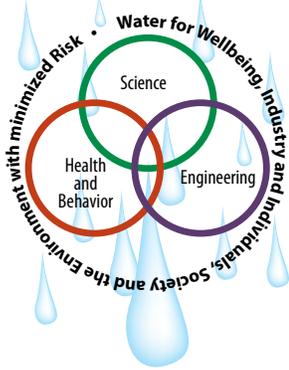


SUSAN DUNCAN • PROFESSOR,
FOOD SCIENCE AND TECHNOLOGY
(540)231-8675 • duncans@vt.edu



Water for Health

Where IGERT Will Take Us

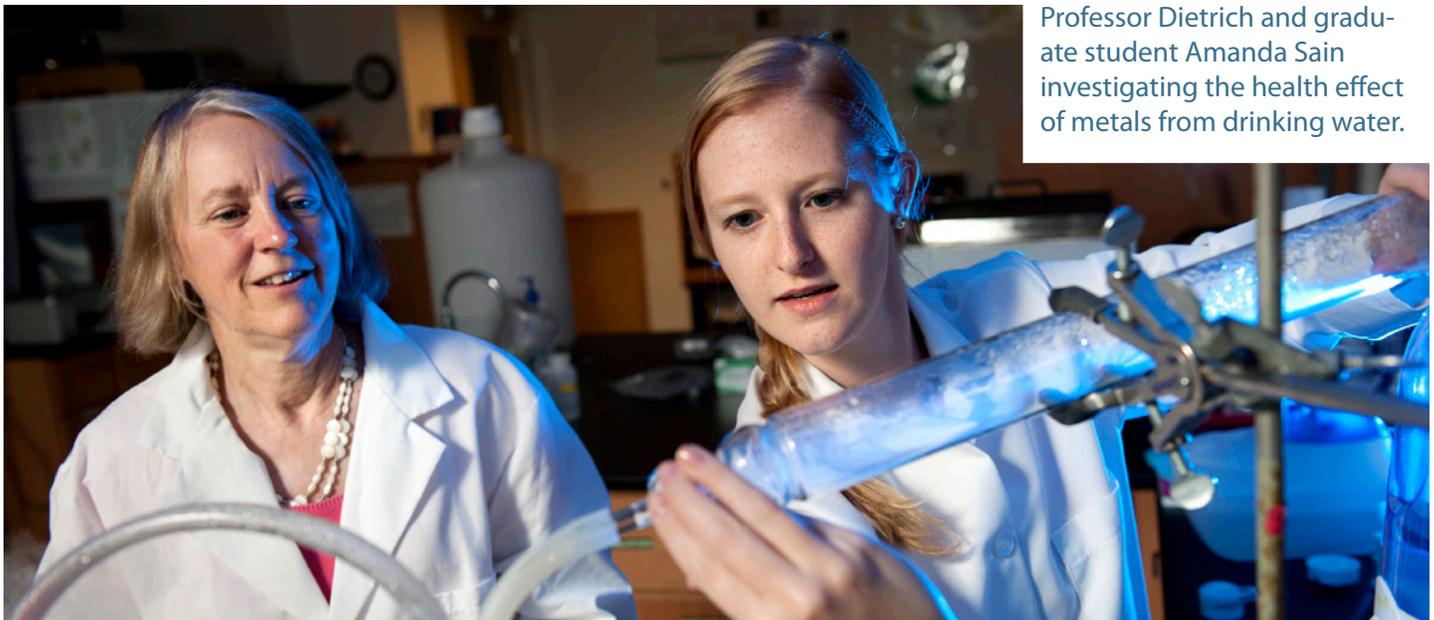


Seed funding from ICTAS sparked the Water for Health initiative which promotes human health and environmental sustainability. A team of interdisciplinary researchers—Andrea Dietrich (Civil Engineering), Brenda Davy (Human Nutrition, Foods and Exercise), and Susan Duncan (Food Science and Technology)—are working together on a range of projects that make tap water a desirable beverage of choice for consumers, thus improving health without the costs and consequences of many

other beverages. To date the team has addressed the role of tap water in diet and obesity, metallic taste sensitivity in patients, and iron nutrition. The research team demonstrated that when adults consume one or more glasses of water at least 30 minutes before a meal, they consume fewer calories and still do not feel hungry. In this way, drinking more water has the ability to keep a person hydrated and to minimize obesity. That work led to the development of a beverage intake questionnaire for evaluating the quantity of tap water consumed amongst all beverage choices and allowed researchers to track habitual water and beverage intake in future research.

Drinking water should have a balance of minerals which provide good flavor and feeling in the mouth. An imbalance of minerals or lack of minerals in liquids such as distilled water can result in an unpleasant astringent or drying taste. Patients receiving medical treatments sometimes experience strong metallic tastes that contribute to a poor quality of life, and these researchers identified a lack of certain salivary proteins that increase sensitivity to elevated copper or iron sometimes present in water. Removal of these metals with standard water treatments can stop the bad tastes. Other research demonstrated that people younger than 50 years of age and individuals with a heightened sense of smell can sometimes find iron in water distasteful. Because too little iron in a diet can cause anemia and too much iron can cause disease, the work is helpful to individual consumers seeking balanced iron intake. Besides enhancing human health, this research helps support consumption of tap water as a more sustainable choice than bottled water.

The Water for Health initiative has also seeded related lines of research that aim to ensure that tap water is safe and free of germs that cause disease, such as Legionnaire's disease.



Professor Dietrich and graduate student Amanda Sain investigating the health effect of metals from drinking water.



Brittany Balhouse

Advisors: Dr. Pavlos Vlachos and Dr. M. Nichole Rylander

Academic Interests: Biomedical Engineering and Sciences; plans to continue her research in Biomedical Engineering working on a 3D tumor platform to examine the fundamental behaviors of

various types of cancer under varying microenvironmental conditions.

Previous Work: B.S. in Biomedical Engineering from North Carolina State University. During her undergraduate career at NC State, Brittany was involved in research characterizing the structural and mechanical properties of porcine heart valve tissue. She also was a 2011 Pratt School of Engineering REU Fellow at Duke University and studied senescence and proliferation in aging endothelial progenitor cells.

Personal Interests: Enjoys snow skiing and playing guitar.



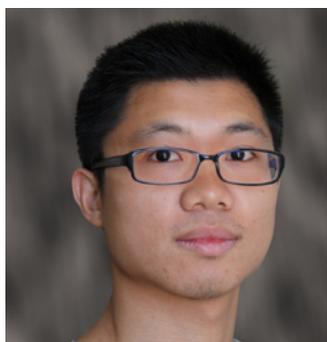
Sallie Beth Johnson

Advisor: Dr. Paul Estabrooks

Academic Interests: Human Nutrition, Foods, and Exercise at Virginia Tech with a concentration in Behavioral and Community Science; current research involves participating in the new Translational Obesity Research

interdisciplinary graduate education training program to tackle the complex societal problem of obesity from a “cells to society” approach, focusing on implementing and disseminating effective obesity prevention and treatment programs on a broad scale to have a positive public health impact.

Previous Work: B.S. in Education from Mount Saint Mary’s College in Emmitsburg, Maryland, and a Master of Public Health (MPH) from West Virginia University, School of Medicine, as well as a Gerontology Certificate from Delaware Technical & Community College in Georgetown, Delaware. She previously served as a Health Educator at FirstHealth of the Carolinas Community Health Services in Pinehurst, North Carolina, and a Research Assistant at the West Virginia University Prevention Research Center in Morgantown, West Virginia. She is also a Master Certified Health Education Specialist (MCHES) and has obtained a Tobacco Treatment Specialist (TTS) certification from the Mayo Clinic.



Xiangtao Meng

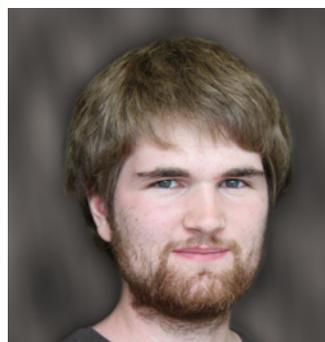
Advisor: Dr. Kevin Edgar

Academic Interests: Macromolecular Science and Engineering Program at Virginia Tech; current research interests focus on synthesis and characterization of novel cellulose derivatives and their potential application in

drug delivery.

Previous Work: B.S. in Pharmacy at Shandong University, China, in 2009 and M.S. in Pharmaceutical Chemistry from the Institute of Oceanology, Chinese Academy of Sciences 3 years later. His Master’s research was focused on synthesis and characterization of chitosan for antibacterial application, from which he published one research article and issued two patent applications.

Personal Interests: Enjoys reading various styles, including novels, fiction and prose, watching animated movies, basketball, and hiking.



Sebastian Mergelsberg

Advisor: Dr. Patricia Dove and Dr. Biswarup Mukhopadhyay

Academic Interests: Geosciences at Virginia Tech; current research focuses around the biological control over biomineralization and how this trait may have evolved, particularly in ter-

restrial crustaceans.

Previous Work: Received his Bachelor’s degrees in Geology and Biology at Rensselaer Polytechnic Institute in 2012. As part of his undergraduate studies, Sebastian worked in the lab of Dr. Bruce E. Watson at RPI for the New York Center for Astrobiology. The research project was aimed at determining the stability of different chemical/isotopic biosignatures in minerals. Preliminary results of this project were presented at the 2012 Goldschmidt Conference in Montreal, QC, in July 2012.



Laura Schoenle

Advisors: Dr. Ignacio Moore and Dr. Fran Bonier

Academic Interests: Biological Sciences; her research focuses on ecology, physiology, and understanding how organisms make life history decisions, including studying the ways that disease

and environmental stressors influence how birds allocate resources towards survival and reproduction.

Previous Work: Received a Bachelor's degree in Animal Science from Cornell University in 2006. After spending time as a field assistant in Australia and a veterinary technician in Tucson, Arizona, she completed a Master's of Education at the University of Arizona. Laura taught high school biology and environmental science for 4 years before moving to Blacksburg, Virginia.

Personal Interests: Enjoys outdoor activities like running, hiking, and bird watching or staying indoors with her two cats.



Craig Schillaber

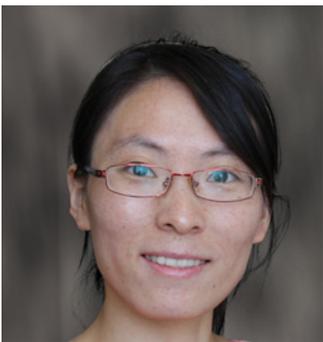
Advisors: Dr. Joseph E. Dove and Dr. James K. Mitchell

Academic Interests: Geotechnical program of the Department of Civil and Environmental Engineering at Virginia Tech; current research involves investigating ways to enhance the sustainabil-

ity of geotechnical design and construction, with a current focus on energy consumption associated with geotechnical ground improvement.

Previous Work: Received his Bachelor's degree in Civil Engineering from the University of New Hampshire and his Master's degree in Civil Engineering from Virginia Tech. After completing his Master's degree, he practiced geotechnical engineering for 2 and a half years at a large private consulting firm in New York City. During that time, Craig worked on some major projects including the World Trade Center and New York City's Second Avenue Subway.

Personal Interests: Enjoys hiking, boating, and pursuing growth in his Christian faith through involvement with his church and the Graduate Christian Fellowship on campus.



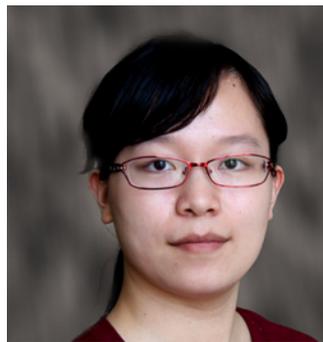
Hua Xiao

Advisors: Dr. Richard Veilleux and Dr. Mark Williams

Academic Interests: Horticulture

Previous Work: Received a Bachelor's degree in Biological Science from Hainan Normal University in China and her Master's

degree in Zoology from Beijing Normal University in China.



Ruoxi Yuan

Advisors: Dr. Liwu Li and Dr. Ansar Ahmed

Academic Interests: Biomedical and Veterinary Sciences through the Virginia-Maryland Regional College of Veterinary Medicine; current research interest is focused on the innate im-

mune responses induced by Lipopolysaccharide (LPS) and monophosphoryl lipid A (MPL).

Previous Work: Received her Bachelor's degree in Bioengineering from Nanjing Agricultural University. During her undergraduate studies, she focused on genetic engineering and molecular biology.

Personal Interests: Enjoys drawing, traveling, and birding.



Virginia Tech's StREAM Lab: A "Common" for Interdisciplinary Research, Education, and Outreach Related to the Dynamics of Water and Societal Systems

The need for sustainable management of water resources at local, regional, and global scales has been identified as one of the key challenges of the 21st century. The world's population is predicted to expand from 6.5 billion to 9.1 billion between 2005 and 2050, creating unprecedented strains upon our natural resources that must be addressed via innovative new approaches. The majority of projected population growth will occur in high-density urban areas, which will simultaneously drastically change land-use ecology while exerting extreme demands for clean water supplies and increased agricultural production. The dynamics of Earth's freshwater processes, though essential for humans and natural ecosystems, are extremely complex.

The Virginia Tech Stream Research, Education and Management (StREAM) Lab is a unique, world-class research center focused on understanding the interactions of natural and human systems. The intense upland urban and agricultural influences on the natural Stroubles Creek watershed system provide an ideal setting for downstream observations of the effects of further human development, stormwater management, and community stewardship behavior on water quality and aquatic ecology. StREAM Lab provides faculty and students with unique opportunities to concurrently conduct research, education, and outreach activities within a few kilometers of campus.

Over 14 courses at Virginia Tech across four colleges have used the StREAM Lab in various field and laboratory exercises, and findings generated at the site are being communicated locally and nationally through tours, stream restoration workshops, the project web site, extension outreach, and peer-reviewed publications. A sample of the wide variety of ongoing research efforts currently within StREAM Lab include:

- **National Science Foundation (NSF) Research Experience for Undergraduates (REU) Site** focused on *Dynamics of Water and Societal System* (led by Drs. Cully Hession and Leigh-Anne Krometis in Biological Systems Engineering).
- **ICTAS Transformative Science and Technology Seed (TSTS) Project** on *Examination of Critical Watershed Processes Governing Dissemination of Agricultural Sources of Antibiotic Resistance* [led by Drs. Amy Pruden (Civil and Environmental Engineering), Katharine Knowlton (Dairy Science), Kang Xia (Crop and Soil Environmental Sciences), Leigh-Anne Krometis (Biological Systems Engineering), and Cully Hession (Biological Systems Engineering)].
- **U.S. Department of Agriculture Agricultural Research Service Grant** to *Use Rare Earth Elements as a Tracer to Understand Sediment Fate and Transport in Small Streams* [led by Drs. Kevin McGuire (Forest Resources and Environmental Conservation) and Cully Hession (Biological Systems Engineering)].
- **National Science Foundation Directorate for Undergraduate Education Grant** for *Integration of Remote Water Sustainability Lab to Enhance Undergraduate Engineering Education* [led by Dr. Vinod Lohani (Department of Engineering Education)].

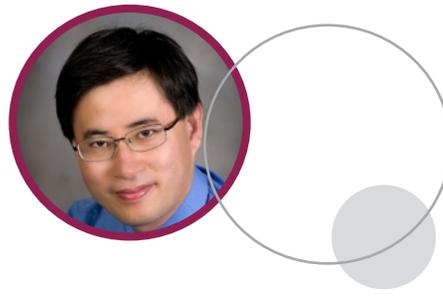


StREAM Lab NSF-
REU Fellows 2012.

DID YOU KNOW?

Stroubles Creek originates from three springs in the Town of Blacksburg, Virginia. These springs form streams that flow through the Town of Blacksburg and the Virginia Tech campus and ultimately merge to form the Virginia Tech Duck Pond. The stream below the Duck Pond dam is known as Stroubles Creek. It flows through Virginia Tech farms, rural areas in Montgomery County, and eventually drains into the New River. The entire Stroubles Creek watershed system is situated within the Mississippi River Basin.

BINGYU ZHAO
ASSISTANT PROFESSOR, HORTICULTURE
(540)231-1146 • bzhao07@vt.edu



Switchgrass Molecular Breeding Program Seeks to Reduce Oil Dependence

Using bioenergy to reduce the oil dependence of the United States is a national priority because of ever-increasing crude oil prices and environmental pollution concerns. Among all forms of bioenergy, biomass-based biofuels have garnered significant attention. Switchgrass is a C4 perennial grass being investigated as a major biomass feedstock for renewable bioenergy production. The four main advantages of a switchgrass energy production system are: (1) high photosynthesis efficiency with high productivity compared with other herbaceous species, (2) a perennial nature that requires minimum management with less consumption of both energy and agrochemicals, (3) established harvesting and storage strategies compatible to the current forage hay production and harvesting system, and (4) an exceptional deep root system that allows

growth on marginal lands that cannot be used for growing food crops. In addition, switchgrass has a large underground biomass (roots) that enhances carbon sequestration in the soil and thus substantially reduces greenhouse gas in the atmosphere. Currently, switchgrass biomass yields range from 4 to 7 tons of dry biomass depending on the cultivars, growth conditions, and management practices.

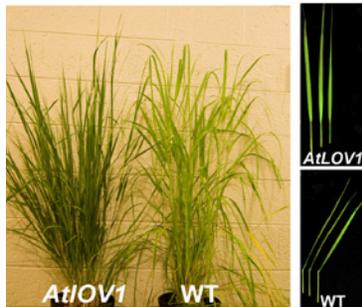
The U.S. Departments of Agriculture and Energy's Billion Ton Study proposed to replace approximately 30% of the nation's current gasoline consumption with biomass-based biofuels by 2030 on a sustainable basis without converting U.S. croplands to switchgrass production. To meet this challenge, switchgrass biomass yields must at least be doubled to produce about 1.3 billion tons of biomass per year from available marginal lands across the nation.

ICTAS-supported Dr. Bingyu Zhao, whose major research area is biotechnology and the genomics of biofuel feedstocks, has established a switchgrass molecular breeding program that employs both traditional plant breeding and genetic engineering methods to improve switchgrass biomass yields. For his breeding program, Dr. Zhao and his research group selected elite switchgrass germplasm from across the U.S. consisting of approximately 2,000 plants representing 168 core germplasm lines. These plants were established in a field breeding nursery at Virginia Tech's Kentland Farm

Station. Since 2007, Dr. Zhao and his research group evaluated these plants for biomass yields and resistance to abiotic and biotic stresses. Zhao's research group also identified a lowland cultivar--Alamo--and an upland cultivar--Dacotah--which are highly divergent for biomass yield, rust resistance, flowering date, lignin content, and drought and cold tolerance. These two cultivars were crossed to generate a population for genetics studies. The Zhao research group also devised an efficient plant tissue culture and genetic transformation system that allows genetic engineering of switchgrass plants with desirable biofuel traits. For example, Dr. Zhao and his research group recently developed a novel switchgrass line through tissue culture selection. The new switchgrass line is significantly taller than the most popular switchgrass cultivar--Alamo.

The group also employed genetic engineering to create a switchgrass plant line with a 25% reduction in the lignin content of the cell wall biomass, a feature which makes this switchgrass plant line 57% more efficient in biofuel production. The Zhao research group also developed switchgrass plants with erect leaves that may allow farmers to grow switchgrass using a higher planting density without compromising the plant's photosynthesis efficiency.

In collaboration with Dr. Brian Lattimer's research group in Virginia Tech's Department of Mechanical Engineering, Zhao's research group will screen different switchgrass germplasm to identify a more suitable cultivar for co-firing with coal in the established combustion system. For details on this collaboration, see "Blending Fuels for Improved Power Production," page 22.



Zhao-developed switchgrass plant (left) with erect leaves.



Zhao-developed novel switchgrass line grows taller than most popular switchgrass cultivars.

JERZY NOWAK • PROFESSOR EMERITUS OF HORTICULTURE
(540)231-2663 • jenowak@vt.edu

JOSEPH L. GABBARD, JR. • RESEARCH ASSISTANT
PROFESSOR, VIRGINIA BIOINFORMATICS INSTITUTE
(540)231-3559 • jgabbard@vt.edu



ICTAS Grant Supports Sustainable Agriculture and Smart Farming

Using Emerging Engineering Technology to Enable Sustainable Agriculture

In the coming years, unprecedented investment will be made in sustainable technologies and practices that impact critical resources such as energy, food, and water. One obvious opportunity to positively manage and impact these resources exists in agriculture where the production of sustainable energy crops like warm season grasses, as well as regional foods, must be managed in ways that improve water quality. Traditional agriculture methods typically are not sustainable and may negatively affect water quality. For this reason, an infusion of engineering technologies is needed to fully realize the economic and social benefits promised by sustainable practices—especially since many agriculture activities rely on limited or dated technologies.



Subsurface microirrigation system delivers water, air, nutrients, pH correction, and other compounds in precise combinations to stressed areas of the ICTAS research plot.

The Smart Farm Project, located at Virginia Tech's Catawba Sustainability Center, contained several intertwined thrusts, each of which introduced its own challenges and merited its own resources and attention. By integrating engineering, horticulture, agriculture, and outreach into a hybrid research and applied setting, we laid the groundwork for future funding, provided a technology platform and research testbed for both graduate and undergraduate research, and supported a local underserved refugee community of Somali Bantu farmers from Roanoke, Virginia. Our work established and integrated a technology platform employing in-ground sensor suites that communicate with mobile hand-held devices similar to an iPhone to report real-time soil conditions that indicate a crop's stress status and thereby drive sustainable agriculture management decisions. Water, air, nutrients, pH correction, and other compounds can be delivered precisely in the stress zone(s) using a subsurface microirrigation system. This platform was fielded in a real-world agriculture production setting where we collected valuable seed data while supporting farmers from the Bantu refugee community. We concentrated our resources on extending the technology platform to include prototype greenhouse gas sensors and finalizing data collection for publication.

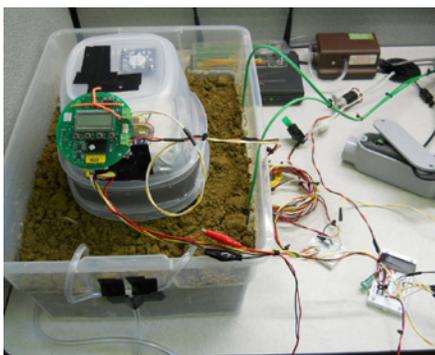
Our work in sustainable agriculture involves four areas: business development, sensor networks, precision irrigation research, and visibility and outreach.

Business Development: Christy Gabbard, Director of Virginia Tech's Catawba Sustainability Center, serves as our coprincipal investigator and is partnering with the Board of Somali Bantu in Roanoke, Virginia, the Virginia Cooperative Extension, and Virginia Tech's Pilot Street Project to train Bantu refugees to produce vegetables and flowers and to educate them about our state-of-the-art engineering technology for soil management. The Bantu farmers grew their crops on an ICTAS research plot and sold their products at the local Roanoke and Catawba farmers' markets.

Sensor Networks for Sustainable Agriculture: Our sensor network consists of 12 solar-powered nodes, each capable of serving four independent sensors that communicate over an ad hoc network to a persistent database. This data can then be viewed and data mined via a local network using mobile devices. The engineering network infrastructure, as well as research issues related to data flow, reliability, and storage,

provided the context for both graduate and undergraduate research that included students from Virginia Tech's Computer Science and Horticulture departments.

We extended our technology platform to include nitrous oxide sensors to quantify reduction in greenhouse gas emissions resulting from our subsurface, forced-aeration irrigation practices. Specifically, under anaerobic soil conditions—that is, when there has been a large amount of rain—soil microorganisms begin to reduce soil nitrogen which results in the production of nitrous oxide. As one of four principal greenhouse gases, nitrous oxide, over the next 100 years, has a Global Warming Potential 298 times greater than that of carbon dioxide and 12 times greater than that of methane. Additionally, current estimates suggest that 50 to 70% of applied nitrogen fertilizer is never taken up by crops under traditional agriculture practices, representing a massive nitrogen source for reducing soil nitrates to nitrous oxide.



Nitrous oxide sensor used to quantify reduction in greenhouse gas emissions.

Our capacity to monitor and compare nitrous oxide losses from aerated and nonaerated production plots enables development of unique, forward-looking solutions for substantially reducing greenhouse gas emissions from arable lands, while at the same time reducing production costs through an increase in nitrogen fertilizer use efficiency and a reduction in plant distress that enables increased yields.

Precision Irrigation: We refined and tested our technology platform to ensure precise delivery combinations of liquids and fertilizers to specific areas of the half-acre ICTAS research plot. This precision irrigation allows us to apply a wide array of experimental designs to various crops, something that cannot be done in a lab, and, to the best of our knowledge, is novel in that it incorporates subsurface irrigation coupled with real-time soil sensors. The research plot consists of 16 rows, each 165 feet long, arranged in blocks of four (for statistical repetition), with source subsurface irrigation lines plumbed such that treatments are counterbalanced using a 4x4 Latin square.

To explore potential greenhouse gas reduction, we incorporated electronic control of a high-volume, low-pressure air pump into our technology platform. Air was injected into a specific set of subsurface irrigation lines to aerate the soil directly after a heavy rain event (when greenhouse gases are typically emitted). We collected data to examine under what specific soil conditions air should be injected, for how long, and what effect this injection has on various crops.

Visibility and Outreach: The Virginia Tech Catawba Sustainability Center, created in 1988 from a gift of 377 acres from the Catawba Hospital, showcases research and demonstration projects from various Virginia Tech colleges, allows university engagement with the local community, and provides a place to practice and learn about sustainability issues. The interdisciplinary nature of the work undertaken here, as well as Virginia Tech's collaboration with the Somali Bantu, has created visibility and outreach opportunities for ongoing individual projects, Virginia Tech, and ICTAS. Another outreach opportunity will occur when the soil sensors demonstrated at the Catawba Sustainability Center are introduced into the science classes offered by Roanoke County Public Schools.



One of 12 solar-powered nodes that enable data collection by the sensor network.

Moving Forward

In July 2012, we added a new member to our team, Dr. Mark Williams, a rhizosphere biologist in Virginia Tech's Horticulture Department. His expertise will help us examine how microbial communities assemble and function in soil ecosystems and root-zone habitats—with implications for both human health food crops. We also have been working to physically and conceptually extend our technology platform to leverage other ongoing interdisciplinary efforts. The synergistic activities described below will position us for broader research funding opportunities.

Urban Horticulture Center: Our technical successes at the Catawba Sustainability Center have positioned us to transition our work to a location closer to campus. We are preparing a new research plot at the Urban Horticulture Center located along Price's Fork in Blacksburg. This location has a well-established infrastructure, and its proximity to campus will afford more interaction with undergraduate and graduate students. We began site selection and soil preparation for the transition in the summer of 2012.

Undergraduate Research Autonomous Robot: Co-PI Nowak and Ph.D. student Jon Weekly are extending a previously successful relationship between the Mechanical Engineering and Horticulture departments. Specifically, with mechanical engineering faculty Dr. Al Wicks, a team of undergraduate mechanical engineering students will engage in a capstone course to design an autonomous robot that will "work in the field" and facilitate our goal of sustainable agriculture through precision delivery of inputs. The autonomous robot will plug into our technology platform and provide additional communication, sensor, and digital image capabilities. This mechanical engineering capstone class started in Fall 2012 and will run through Spring 2013. The timing is fortuitous, as we work to keep our momentum going, and look to extend the capabilities of our technology platform.



MICHAEL F. HOHELLA, JR
 VT SUN DIRECTOR,
 UNIVERSITY DISTINGUISHED
 PROFESSOR, GEOSCIENCES
 (540)231-6227
 hochella@vt.edu



LINSEY C. MARR
 ASSOCIATE PROFESSOR, CIVIL
 AND ENVIRONMENTAL ENGI-
 NEERING
 (540)231-6071
 lmarr@vt.edu



SEAN MCGINNIS
 DIRECTOR OF VT GREEN
 ENGINEERING PROGRAM,
 ASSOCIATE RESEARCH
 PROFESSOR, MATERIALS SCIENCE
 AND ENGINEERING
 (540)231-1446 • smcginn@vt.edu

Sustainable Nanoenabled Consumer Products

The Woodrow Wilson International Center for Scholars' (WWICS) Nanotechnology Consumer Products Inventory (NCPI) provides an important resource for numerous nanotechnology stakeholder groups ranging from consumers to researchers and policy developers. Despite having nearly 200,000 unique visitors since 2008, and dozens of citations in peer-reviewed publications and grant proposals, a critical limitation of the NCPI has been its reliance on manufacturer claims to justify product listings. In 2011, the ICTAS-supported Virginia Tech Center for Sustainable Nanotechnology (VT SuN) and the Project on Emerging Nanotechnology (PEN) at WWICS initiated a unique University/NGO partnership to implement several critical modifications to the inventory (www.nanotechproject.org/inventories/consumer). These modifications complement manufacturer claims and improve the utility of the NCPI among a growing number of stakeholders who rely on this resource for increasingly diverse and sophisticated uses. Modifications to the NCPI include categorizing products based on science-driven information, integrating Life-Cycle Assessment (LCA) input/output databases for improved analysis and decision-making, creating an open users community to facilitate information sharing, establishing a technical oversight and governance committee, and developing embedded traineeships that leverage the inventory to foster new interdisciplinary research projects at the interfaces between nanoscale science and engineering, consumer product safety, sustainability, and science and technology policy decisions. With the combined scientific expertise of VT SuN and the Virginia Tech Green Engineering Program, this new partnership with PEN provides a unique opportunity to address the inherent limitations of the NCPI as it was originally designed and to enhance its scientific credibility to provide consumers, policymakers, and researchers with the credible information they need to make informed decisions about nanotechnology products.

Sustainable Nanomaterials in Consumer Products

Nanotechnology offers many opportunities for the development of new products

and technologies across a wide spectrum of applications. Nanomaterials are defined as materials that have one or more dimension less than 100 nanometers (nm). Scientists and engineers are focused on nanomaterials because their enhanced materials properties lead to superior product performance. Properties of nanomaterials are particularly size dependent, allowing engineers and scientists to tailor properties in ways not available using current macro-sized materials. Examples of nanomaterials in consumer and commercial products include nanosilver for antibacterial applications, nanotitanium for use in cosmetics, carbon nanotubes for structural applications, nano-optical devices for sensors, nanoelectronics for computers and other "smart" devices, medical diagnostic tools, and nanoclays for food applications.

Because there is so much potential for these novel materials, the science and engineering of nanotechnology is progressing faster than is our understanding of the implications of their use. Thousands of products containing engineered nanomaterials are available in the marketplace, and this number is expected to grow dramatically as the technology matures. These nanomaterials are currently unregulated for most applications, yet the value of the products and goods that they are in will soon exceed one trillion dollars annually.

An emerging concern is the environmental and human impacts of nanomaterials. Recent studies indicate that, in some cases, there is a possibility of damage to ecosystems and human health from these novel materials. The ICTAS research thrust in Nanoscale Science and Engineering is actively researching several aspects of the environmental impacts and sustainability of nanomaterials in consumer products.

One research avenue is a collaboration between VT SuN, the WWICS, the University of Michigan Risk Science Center, and the WWICS Project for Emerging Nanotechnologies (PEN). This project is "dedicated to helping ensure that as nanotechnologies advance, possible risks are minimized, public and consumer engagement remains strong, and the potential benefits of these new technologies are realized"

(<http://www.nanotechproject.org/inventories/consumer>).



ERIC W. VEJERANO
 POSTDOCTORAL ASSOCIATE,
 DEPARTMENT OF CIVIL &
 ENVIRONMENTAL ENGINEERING
 ENVIRONMENTAL
 PROGRAM
evejer1@vt.edu



MATTHEW S. HULL
 PROGRAM MANAGER, ICTAS
 (540)231-5812
mahull@vt.edu



TOM EWING
 ASSOCIATE DEAN,
 GRADUATE STUDIES AND RE-
 SEARCH, COLLEGE OF LIBERAL
 ARTS AND HUMAN SCIENCES
 (540)231-3212
etewing@vt.edu

Utility of the Nanotechnology Consumer Products Database

One of VT Sun's goals is to create and/or adapt categorization schemes to increase the utility of the NCPI database for various stakeholders. We have added new categories to the database describing the identity, form, and location of nanomaterials within products, possible exposure routes of the nanomaterials, and finally the likelihood of exposure. Identifying the locations of the nanomaterials, whether clustered on the surface of products or evenly distributed throughout, is an important initial step in assessing possible routes of exposure to humans or release into the environment during the products' use and disposal. Possible exposure routes were determined as inhalation, oral, and dermal, or a combination of these. So far, the majority of ~300 products that have been assessed to date are expected to cause exposure, especially products belonging to the health and fitness, automotive, and home and garden product categories, as depicted in Figure 1.

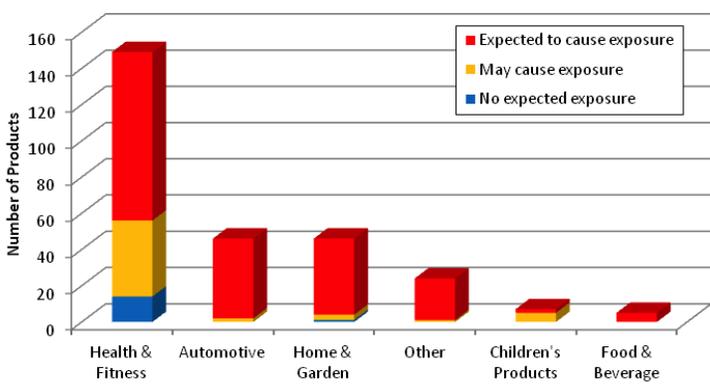


Figure 1. Exposure risks of nanomaterials from various product categories.

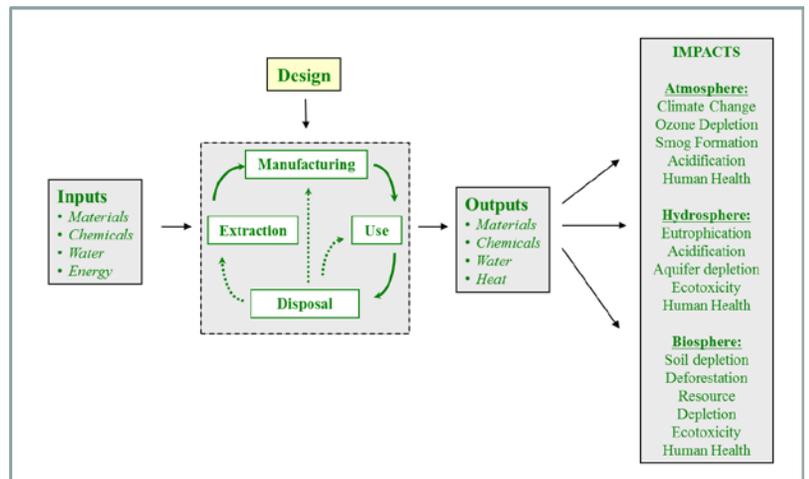


Figure 2. Life-Cycle Assessment General Methodology.

Virginia Tech Green Engineering Program

The VT Green Engineering Program is also working through the ICTAS Nanoscale Science and Engineering Research Thrust to consider the life-cycle environmental impacts of nanomaterials incorporated into consumer products. All materials have environmental impacts across their life cycle. Raw materials must be extracted, transported, and manufactured into usable forms. These steps require energy, chemicals, and water and emit waste into the air, water, and soil. In the use phase, products may require additional energy and chemicals. At the end of useful life, products enter the disposal phase which typically means landfilling or incineration.

The main difference for the life-cycle environmental impacts of nanomaterials is the level of uncertainty in this area. The field of life-cycle assessment (LCA) has for several decades been refining the methodology to quantitatively estimate overall impacts over a range of environmental categories. Figure 2 is a schematic of the LCA methodology. LCA methods require an inventory of all inputs and outputs for a product/process. Of particular concern are actual nanomaterial outputs during

Continued on back cover

LAURA M. REESE • PHD STUDENT
SCHOOL OF BIOMEDICAL ENGINEERING & SCIENCES

LISSETT RAMIREZ BICKFORD • ASSISTANT PROFESSOR
MECHANICAL ENGINEERING AND
SCHOOL OF BIOMEDICAL ENGINEERING & SCIENCES
(540)231-0622 • *bickford@vt.edu*



Translational Nanomedicine for Healthy Citizens and a Sustainable Future

Ambiguities in translational nanomedicine

Since the emergence of nanomedicine in the early 1990s, interest in this technology has skyrocketed as evidenced by a mass influx of publications and patents. While countless nanoparticles with potential in the healthcare sector have been investigated, roughly 250 nanomedicines are undergoing clinical trials or have received approval for human use from the Food and Drug Administration. Even though this number seems promising, history has shown us that many such candidates fail during clinical trials and that even approved therapies can (and do) get pulled from the market. Why is the number of successful approved products so low considering the commonality of the field? This can be partially attributed to the infancy of nanomedicine; typically the process from initial design and development of devices and drugs through required testing and optimization takes several years. Even after taking into account delays purely caused by regulatory requirements, many favorable products seem to suffer from translational attrition. What are the other obstacles to effectively bringing nanomedicines to market? As with other healthcare inventions, cost-prohibitive designs and formulations, difficulties in scale-up necessary for mass production, and unanticipated toxicities are predominantly responsible for preventing clinical realization. Remarkably, several unanswered questions still remain about the long-term effects of exposure to these nanoscale products in both the environment and in the body. Perhaps the solution to successful translational nanomedicine lies in a more forward-thinking approach—one that involves adapting sustainable practices to the development of nanomedicines at the onset.

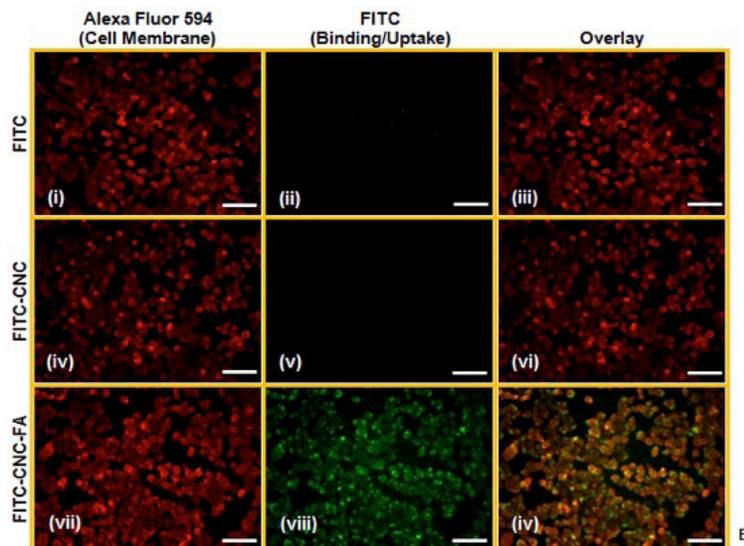
Can we make nanomedicines more sustainably?

The words “going green” tend to conjure up images of recycling and reducing waste in an effort to reduce emissions, lower carbon footprints, and preserve nature. These days, going green and living sustainably seem to be en vogue, and increasingly, many consumers and businesses are caring more about protecting the environment from pollution, toxic chemicals, and unnecessary waste and byproducts.

With the recent boom of nanoscale research and production, which has undoubtedly resulted in many significant and widespread technological advances, concerns for public

health and safety are becoming an area of intensified scrutiny. In fact, a new organization called the Sustainable Nanotechnology Organization has recently been formed and is sponsored by the National Science Foundation as a platform for engineers, scientists, and policymakers to focus on sustainable nanotechnology. But what is sustainable nanotechnology, and can we apply these practices to research in nanomedicine so that we can create safer and more translatable products?

In an effort to prevent potential negative consequences, sustainable nanotechnology is focused on having a proactive rather than reactive approach to product design and development. In general, this means thinking about the environment and human health at the beginning stages of nanotechnology inception, rather than after the fact—when toxicity and other issues may become uncovered. While sustainable nanotechnology is gaining popularity, one area within this field that has received less attention is nanomedicine. Researchers across the globe are looking at nano-sized solutions for healthcare issues, yet little attention has been paid to making these solutions as sustainable as possible, that is—using green chemistry and green engineering principles to avoid downstream problems that ultimately prevent positively impacting human health.



Selective uptake of folate-conjugated cellulose nanocrystals labeled with FITC (FITC-CNC-FA) to breast cancer cells. Scale bar: 100 μ m. Photo provided courtesy of Katelyn Colacino and Yong Woo Lee, VT

A multitude of nanomedicine applications, such as drug delivery, diagnostic imaging, and biomaterials for medical devices and tissue regeneration, exists in the healthcare sector. Currently, drugs dominate the nanomedicine field. Many of these nanotherapeutics are micromolecules, such as liposomes and certain proteins that have been on the market for decades, which have been redesigned to the nanoscale. The remaining therapeutics utilize metallic or other novel formulations whose short-term biocompatibility is believed to be known but whose long-term toxicity still remains questionable. Two of the most unique attributes of nanoparticles are their distinctive biodistribution and targeting abilities. These small particles are able to disperse in a way that their predecessors were unable to, lending to their increased effectiveness. These new materials, such as specific markers that are overexpressed in tumors, can also be engineered to target different areas within the body. This targeting ability provides a unique drug delivery mechanism that can potentially minimize the amount of drug needed and reduce harm to healthy tissue.

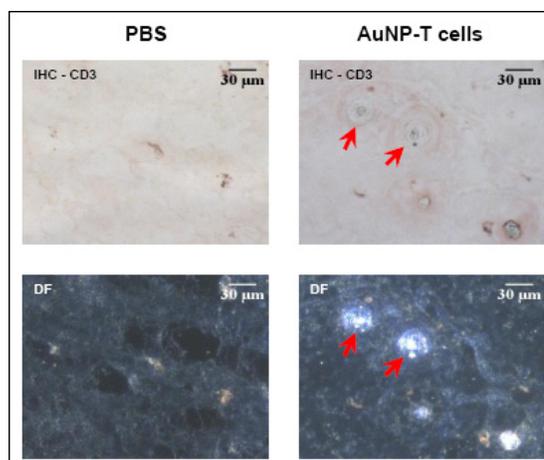
Much research has focused predominantly on solving the medical need first (such as killing cancer cells) with minimal attention being paid to long-term effects. Although the need exists for the nanomaterials to function as intended, the reality is that the translation of these nanomaterials into patient use will come to a screeching halt if the ultimate fate of these products is to cause significant disturbances in the environment or in the patient long after treatment goals have been realized. Perhaps a greener approach would then either evaluate materials that are sustainable to begin with (such as those from plant-based fibers) or would take existing promising candidates and modify their fabrication processes in an effort to make them more sustainable. As efforts in nanomedicine have evolved, there has also been a more recent focus on using more natural products for medicinal use, such as nanoparticles made from spices (like cumin) and biomaterials made with cellulose for tissue scaffolds. Nevertheless, many unknowns exist regarding nano-based products in general, resulting in most of them remaining in the developmental stage until certain questions regarding efficacy, long-term toxicity, and persistence within the human body can be answered. Surprisingly, the mechanisms of transport within the human body at the cellular level and the long-term effects of exposure to nanomedicines still remain largely unknown.

Achieving sustainable and translational nanomedicine

Nanomedicine has many factors that need to be overcome before it achieves widespread translation. In particular, the aforementioned concerns must be addressed. Standard pharmaceuticals stay within the body for a known amount of time before they are metabolized and excreted through the urine. Because of nanoparticles' unique biodistribution, their removal from the body is not completely understood. Many nanoparticles are known to be persistent within the body for months, even years, after administration. This persistence can lead to long-term toxicity. In fact, the majority of therapeutics in preclinical trials are used to treat life-threatening illnesses such as cancer. Some of these drugs have known risks and long-term toxicities, but they proceed to trials because of the nature of the disease they are addressing. This places a limit on the types of diseases that can be treated and could lead to subsequent problems down the road.

Other obstacles that must be overcome for successful translation of nanotechnology includes developing cost-effective solutions and surmounting difficulties in scale-up from low volumes in the lab to industrial-size production. Frequently, when increasing volumes at the nanoscale, certain parameters of the technology, such as monodispersity, size, shape, and drug encapsulation efficiencies, are also altered. This results in increased time and cost in order to reoptimize the materials and processes. With a focus on sustainability during development, the use of safer and more renewable materials for nanomedicine production may correspondingly result in greater cost effectiveness compared to "less green" practices.

To achieve ubiquitous translational nanomedicine, a more holistic approach is needed, and the importance of inter- and multidisciplinary research cannot be overstated. The realization of nanomedicine's universal impact on human health requires an "all hands on deck" mindset where clinicians, basic scientists, engineers, nanotoxicologists, public health advocates, and technology transfer representatives are fully engaged to ensure conscientious nanomedicine development and dissemination of resulting knowledge for the benefit of society. Current nanotechnologies are just barely scratching the surface, and this approach will certainly allow nanomedicine to reach its full potential and truly revolutionize global biotechnology.



Resected mouse tumors analyzed by bright field imaging (top row) and immunohistochemistry for human CD3 expression and dark field imaging (bottom row) to indicate the presence of AuNPs fabricated from a rapid and purification-free carbon monoxide reduction process. Red arrows indicate the co-localization of CD3⁺ T cells and AuNPs within the tumor.

Photo provided courtesy of Joe Young and Rebekah Drezek, Rice University

Reference:

Michael L. Etheridge et al., "The Big Picture of Nanomedicine: The State of Investigational and Approved Nanomedicine Products," *Nanomedicine*, in press (2012).



BRIAN Y. LATTIMER
 ASSOCIATE PROFESSOR,
 MECHANICAL
 ENGINEERING
 (540)231-7295
 lattimer@vt.edu



FRANCINE BATTAGLIA
 ASSOCIATE PROFESSOR,
 MECHANICAL
 ENGINEERING
 (540)231-0077
 fbattaglia@vt.edu



DANESH TAFTI
 PROFESSOR OF ENGINEERING,
 MECHANICAL ENGINEERING
 (540)231-9975
 dtafti@vt.edu

Advancing Coal and Biomass Gasification through Modeling

Power production plants based on the new Integrated Gasification Combined Cycle (IGCC) are being designed to be highly efficient, “zero” emission, and capable of using the nation’s natural resources. In an IGCC plant, gas turbines are fed synthetic gaseous fuel (syngas) produced from solid fuels such as coal and biomass instead of natural gas. Syngas is produced using a gasifier. Gasifiers operate by introducing solid fuel particles such as coal and biomass into a high-temperature, low-oxygen environment resulting in a stream of syngas gaseous fuel consisting mainly of hydrogen, carbon monoxide, and methane. Existing pilot gasifier plants have been found to have reliability issues due to inconsistent syngas fuel stream composition, very restricted solid-

fuel-type input, and excessive maintenance of gasifier construction materials. Scaling small-scale laboratory-size experiments has been problematic in providing solutions to these issues. Methods for bridging the gap between small laboratory-size gasifiers and real-scale power plant gasifiers are needed to advance gasifier design. Advanced computational fluid dynamics (CFD) models can be used to bridge this gap by providing detailed information on conditions inside a gasifier, performance comparison of various gasifier designs, and impact of fuel and operating conditions on the syngas fuel stream.

A multidisciplinary group of researchers, led by ICTAS-supported Dr. Brian Lattimer, has been actively developing advanced CFD models and experimental techniques to support the design approach shown in Figure 1 to assist industry in coal and biomass gasification technology development. In this collaborative effort, detailed and multiscale CFD models are being formulated to provide a full understanding of the behavior in different gasifier designs. Particle details of the gasification process are predicted using a discrete element model (DEM) that simulates the motion and interaction of individual particles within a gaseous flow environment. Because of computational expense, the DEM is used primarily to understand the influence of local conditions on particle behavior. For overall performance of gasifiers, a CFD model known as a two-fluid model (TFM) is used to predict the motion of particles and gases as well as the syngas fuel stream in gasifiers ranging from small-scale to real-scale. Experimental facilities and methods have been developed to support

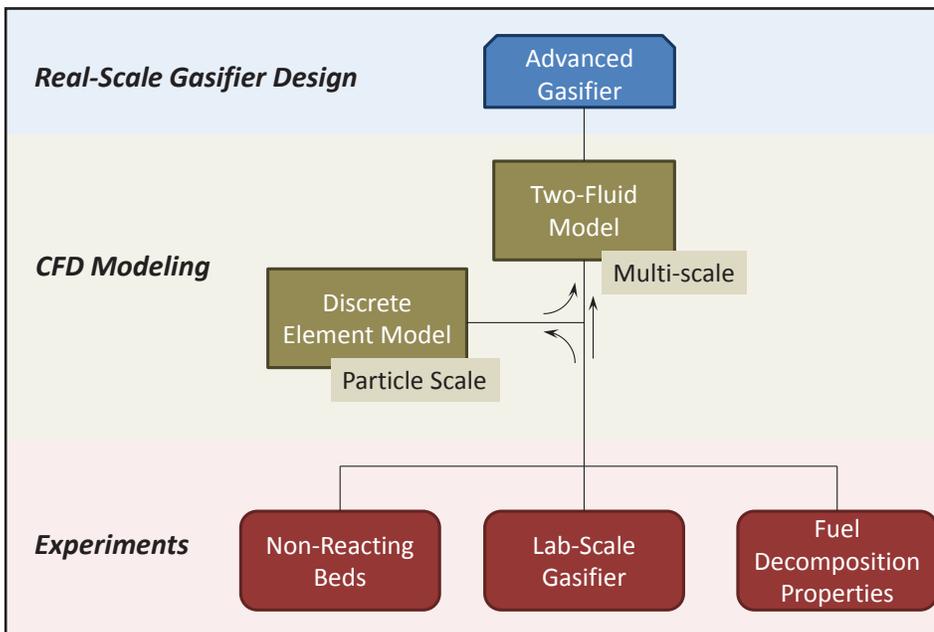


Figure 1. Design approach for advanced gasifier design.



SRINATH EKKAD
 PROFESSOR,
 MECHANICAL
 ENGINEERING
 (540)231-7192
 sekkad@vt.edu



URI VANDSBURGER
 PROFESSOR,
 MECHANICAL
 ENGINEERING
 (540)231-4459
 uvandsbu@vt.edu

validating these models as well as to quantify fuel decomposition characteristics for formulating particle decomposition models to be used in CFD models.

The group has focused on gasification in fluidized beds because of their flexibility in fuel type, but techniques can be applied to other types of gasifiers as well. In typical fluidized beds used for gasification, air is blown through the bottom of the bed through a distributor plate. The bed might consist of coal particles or a mixture of coal and biomass, or fuel particles mixed with a bed material such as sand. Based on the properties of the bed material, once the fluid velocity increases beyond a certain threshold, the bed becomes mobile and behaves like a fluid.

Fluidization should be accompanied by intense and uniform mixing in the bed which is required for efficient operation to avoid nonuniformities in the bed that could lead to hot spots. The design of the distributor plate, the fluidization regime in the bed,

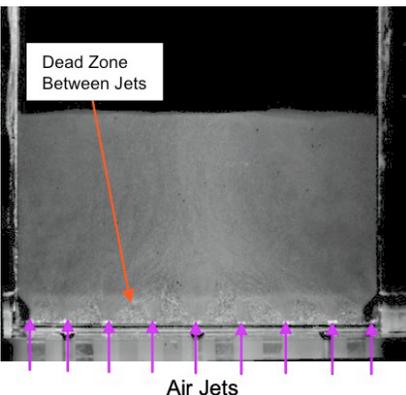


Figure 2. Nonreacting fluidized bed experiment with a nine-gas-jet distributor plate fluidizing spherical glass particles.

the effective mixing between fuel particles of different sizes and densities are some of the quantities of interest.

Experiments on Particle Behavior in Fluidized Beds

Experiments were performed in this research to quantify the effect of gas jet inlet effects on the hydrodynamic motion of particles in a nonreacting bed

shown in Figure 2. In nonreacting experiments, 500- to 750-micron-diameter glass and ceramic particles are used to represent the biomass, coal, or filler that would be used in actual gasifiers. These data were also used to validate CFD models. Noninvasive experimental techniques were used to capture full-field variation of particle/gas distributions, particle velocities, particle temperatures, and heat transfer to gasifier wall surfaces. These measurements were made in a series of small-scale, nonreacting gasifiers with gas jet inlets at the distributor plates for a range of flow regimes including fixed bed, fluidized bed, and spouting bed.

Particle motion and distributions were measured using a Particle Image Velocimetry (PIV) system. These measurements were used to quantify the level of mixing between the particles and the incoming air jets at the bottom of the bed. A comparison of the level of mixing of particles

within the bed is shown in Figure 3 for cases with nine jets and four air jets with the same jet velocity and total air flow rate into the bed. The total mixing rate was 52% higher in the case with nine jets. This higher rate was due to the larger triangular-shaped stagnant regions of particles that form at the bottom of the bed, called dead zones, as the jets become more separated. These dead zones are also highlighted in Figure 2. Reducing the size of these dead zones is important to ensure uniform temperatures within the bed as well as efficient use of fuel particles.

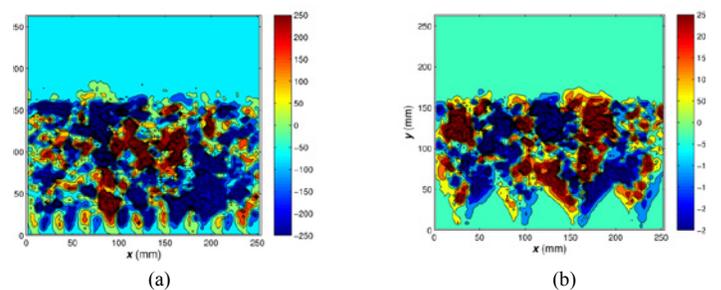


Figure 3. Particle mixing in experiments with a) nine jets and b) four jets.

Heat transfer between the gas jets and the particles as well as to the walls of the fluidized bed are also of interest in gasifier design. An infrared (IR) thermal camera was used to quantify these heat transfer effects. A novel method was developed to quantify heat transfer to the walls of a nonreacting fluidized bed. In this method, inverse heat transfer analysis was performed on temperatures measured using an IR camera image of one wall of the bed constructed of stainless steel foil. Through this analysis, heat fluxes from the bed on the pixel level of the camera were measured. Heat transfer

ADVANCING COAL AND BIOMASS GASIFICATION THROUGH MODELING

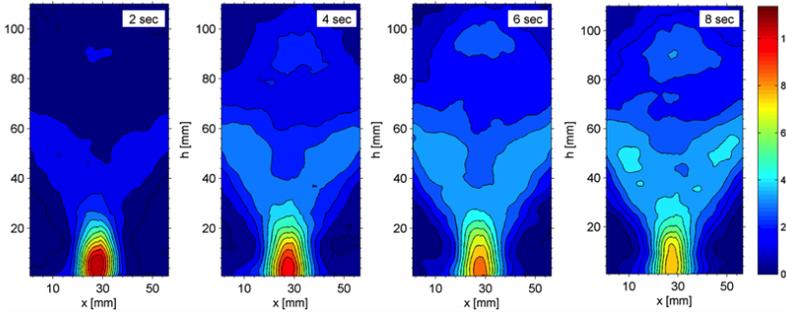


Figure 4. Heat transfer to the wall of a spouted bed with a hot gas inlet.

to the wall of a spouting bed is shown in Figure 4. The highest heat fluxes were measured low in the bed close to where hot gases enter the setup, and later in time high in the bed where particles from the spout fountain re-enter the bed.

Biomass and coal, when sufficiently heated, decompose from a solid into a gas. Predicting this decomposition and the gaseous products of decomposition is essential to accurately modeling a gasifier. All natural materials will decompose differently; therefore, the decomposition characteristics of the fuels of interest need to be measured. As shown in Figure 5, biomass decomposes at lower temperatures and over a more

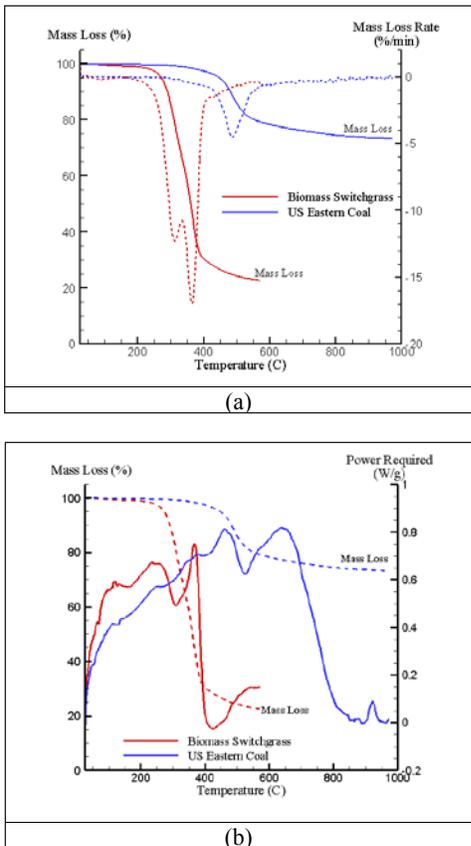


Figure 5. Comparison between coal and biomass a) gravimetric response and b) energy required to heat up and decompose.

narrow temperature range compared with coal. In addition, the energy required to decompose biomass is less. Experimental capabilities also exist to measure the gases produced due to decomposition in low-oxygen environments as well as the potential chemical energy released from these gases to support model development and input.

Particle Scale Modeling

In the DEM, the motion of individual particles is tracked in the bed of particles by solving the dynamical equations of motion. In typical fluidization-based processes, fluid drag, gravitational, and collision forces are important. In the DEM, collision forces are the most challenging to compute. Because the time scales associated with actual collisions are extremely small (in the range of microseconds or less whereas meaningful simulation times extend to seconds and minutes), the simulations model the collision of particles using the assumption of a soft sphere which increases the collision time scale and makes the simulations more tractable. In spite of this, DEM simulations in fluidized beds are computationally intensive, and a few seconds of physical time can take months of simulation time. Thus, the use of large supercomputers and hundreds of processors working together in parallel is necessary to simulate a large system of particles.

DEM has been incorporated into our in-house CFD solver GenIDLEST. The combined DEM-CFD code has been tested extensively with fluidized beds having different distributor plate configurations. Figure 6 shows snapshots of a uniformly fluidized bed with a porous distributor plate. Gas bubbles can be observed in the upper region of the bed, also known as the freeboard region. The bubbles burst at the freeboard and eject particles with high velocities. These particles fall back to the bed because of gravity and form a recirculation pattern for efficient mixing.

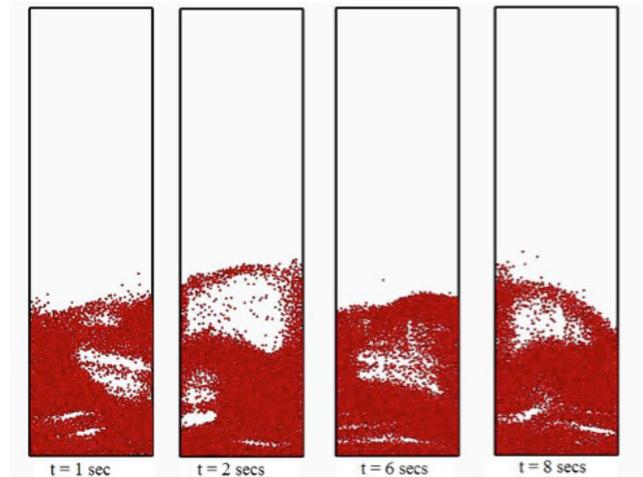


Figure 6. Bubbles forming in a uniformly fluidized bed.

Fluidized beds need not necessarily have distributor plates with uniform pores. Based on industry requirements, they can have distributor plates with slots which lead to jets. Figure 7 shows a typical fluidized bed with a central jet in it. The fluidization characteristics are different for this variation of fluidized beds. It can be seen that instead of large bubbles forming as in Figure 6, the bubbles in this case are smaller and more concentrated at the center of the bed. The top layer of particles has been colored green to show the circulation pattern. A central jet which penetrates through the depth of the bed and gives rise to a single bubble at the freeboard can be seen. Particles on top fall down from the sides and subsequently get entrained in the jet. Finally, a thorough mixing of particles is observed due to this entrainment. Typically, this mixing is desired in industries.

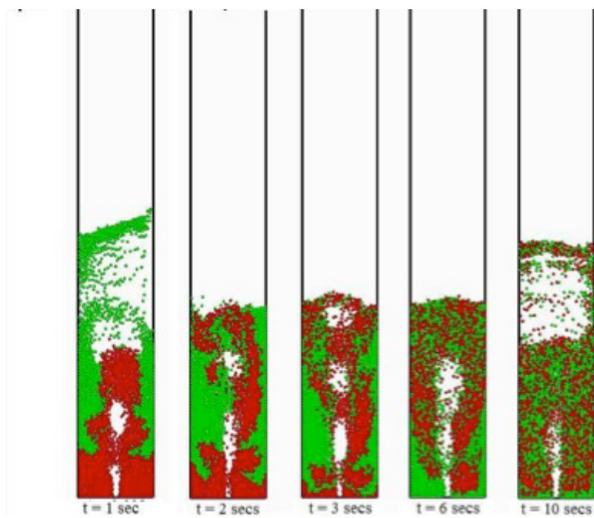


Figure 7. Circulation pattern of particles in a fluidized bed with a single jet.

Along with proper mixing, industries also have the need to separate or segregate particles with different properties (diameter, density, weight, etc.) or in the case of coal and biomass mixtures ascertain uniform mixing and combustion. A fluidized bed with a bimodal mixture (mixture having two different particle diameters) is shown in Figure 8. The particles colored in green are larger and heavier than those colored in red. Because of the difference in weight, the particles tend to segregate and fluidize in groups.

As seen from these results, DEM can elucidate on the detailed physics of fluidized beds and can aid the development of better models for the simulation of large industrial-scale gasifiers planned for use in Integrated Gasification Combined Cycle (IGCC) power plants.

Gasifier Performance Modeling

A gasifier can range in size from tens of centimeters such as in a pilot-scale to tens of meters in a real-scale industrial application. TFM is a computationally more efficient

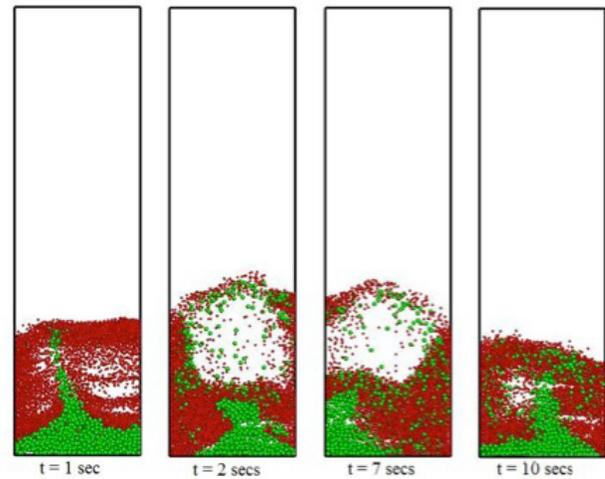


Figure 8. Bubble formation in a fluidized bed with bimodal particle distribution.

CFD modeling approach that can be used to predict gasification over the entire range of gasifier scales. The TFM mathematically describes each gas and solids phase as interpenetrating continua. The governing equations for conservation of mass, momentum, energy, and species are discretized and solved on a computational grid, providing solutions for velocity, temperature, etc. for each phase. In this framework, variables are averaged over large regions with respect to the particle diameter, but the regions are small with respect to the characteristic dimension of the complete system. Closure models are used to describe gas-solid interactions such as drag force models, and mass and heat interphase transfer. The TFM is computationally less expensive but requires more phenomenological modeling of bulk interphase interactions.

The multifluid CFD code known as Multiphase Flow with Interphase eXchanges (MFIx) was used as the TFM in this research and was originally developed by the Department of Defense's National Energy Technology Laboratory (NETL). We have predicted flow characteristics, such as bubble rise velocity in fluidized beds, and particle mixing and particle elutriation, which was compared with experiments. We have also tested and validated drag models to determine which models are capable of predicting the hydrodynamics of a biomass fluidized bed and how to model binary and tertiary systems. Another issue explored was modeling the effects of a real distributor plate, especially because discrete jets create nonuniform fluidization of bed material and introduce regions of high velocity. Even with the TFM, the computational time required for a three-dimensional simulation can be excessive; thus, studies were also pursued to compare the results for two-dimensional (2D) versus three-dimensional (3D) modeling.

Simulations were performed using MFIx to validate 2D and 3D CFD modeling with the experiments of a quasi-2D reactor that used a distributor plate with nine equally spaced holes. For validation of the CFD predictions, pressure drop through the bed was compared with the experimental data, as shown in Figure 9(a). Subsequent to fluidization at 23 cm/s, the linear increase of pressure drop for the experiments suggests en-

ADVANCING COAL AND BIOMASS GASIFICATION THROUGH MODELING

trainment of particles from dead zones that form between the gas jets flowing through the distributor plate. The experiments show that more particles are fluidized with increasing velocity but are less than the total mass of the bed, as suggested by the difference between the theoretical pressure drop across the bed and the experimental values. Figure 9(b) presents the variation of solid volume fraction across the bed width versus a height Z^* (normalized with the initial static bed height, h_0) at an inlet velocity of 35 cm/s. The 2D and 3D predictions are in very good agreement with the experiments.

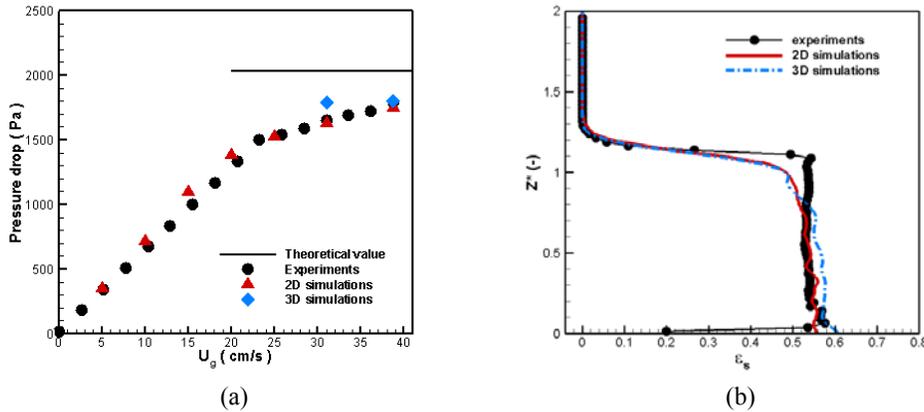


Figure 9. Comparisons between experiments and simulations for (a) pressure drop versus inlet gas velocity and (b) solids volume fraction spatially averaged versus height.

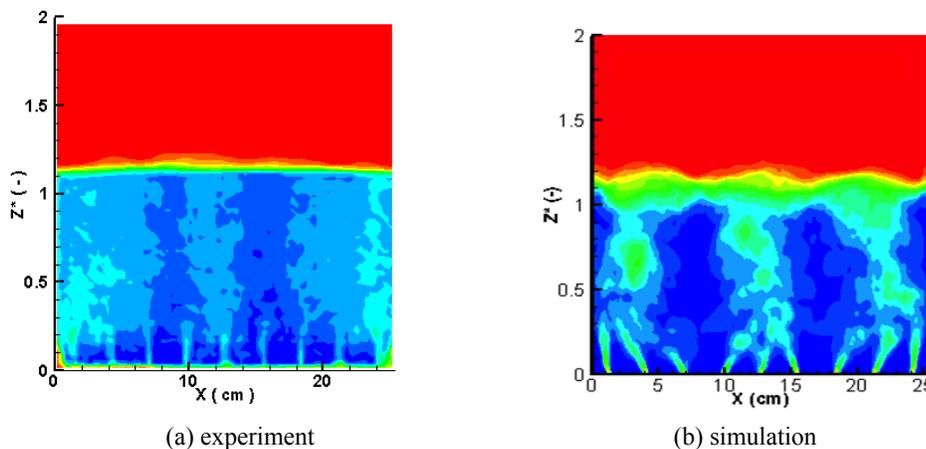


Figure 10. Gas volume fraction for an inlet velocity of 35 cm/s for (a) experiments and (b) simulations corresponding to the distributor plate configuration with nine holes.

As a means to elucidate the complex dynamics of the gas-particle interaction, Figure 10 presents the gas distribution for an inlet gas velocity of 35 cm/s. The experiment shows a fairly uniform gas distribution throughout the bed above $Z^* > 0.2$. The presence of distinct jets diminishes above $Z^* = 0.3$ as the jets coalesce and form bubbles that erupt at the top of the bed. The jet penetration length can also be identified in Figure 10, and the simulation is consistent with that observed for the experiment. In conclusion, the simulations can be considered to be strongly validated. Further validation was performed for different configurations of the distributor plate and different flow rates, and the comparisons were very good.

Concluding Remarks

Models have been developed and validated to support designing more advanced gasifier systems. The TFM model includes combustion of particles, which will be used to validate future planned lab-scale gasifier experiments. Input combustion data for the particles are being developed from decomposition properties of biomass and coal. A lab-scale gasifier is being fabricated for use in validating models with a reacting bed, measuring the behavior of biomass and coal in different operating conditions, and evaluating the impact of blending fuels.

BRIAN Y. LATTIMER

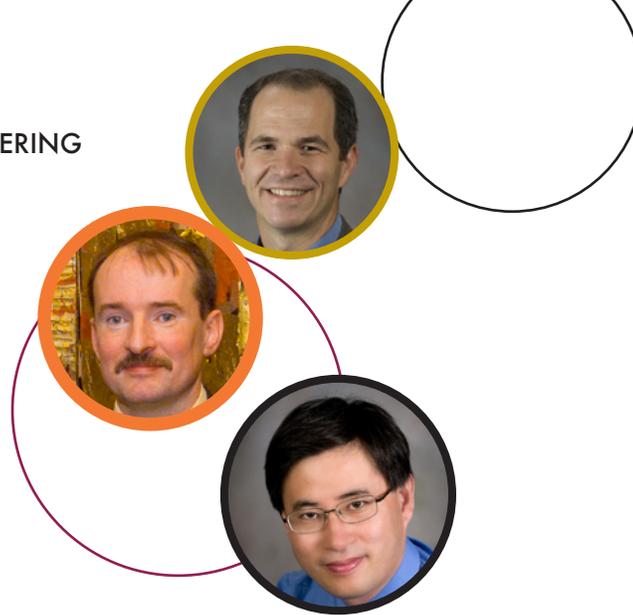
ASSOCIATE PROFESSOR, MECHANICAL ENGINEERING
(540)231-7295 • lattimer@vt.edu

GERALD LUTTRELL

ALPHA NATURAL RESOURCES PROFESSOR,
MINING AND MINERALS ENGINEERING
(540)231-6314 • luttrell@vt.edu

BINGYU ZHAO

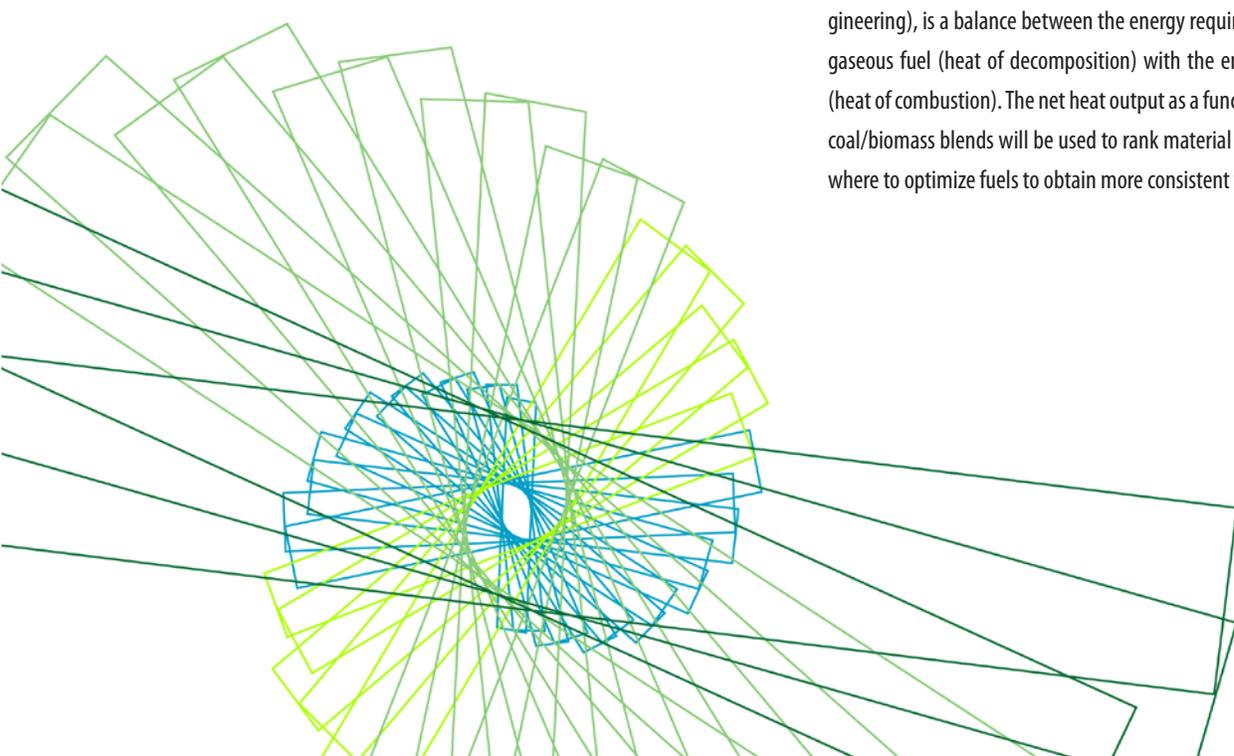
ASSISTANT PROFESSOR, HORTICULTURE
(540)231-1146 • bzhao07@vt.edu



Blending Fuels for Improved Power Production

A variety of methods using solid fuels, each with its own fuel requirements, is available for power production. These requirements may be driven by ash content, operating temperature, heating rate, and feeding process. In all applications, a consistent output fuel stream or power output is desirable. Natural fuels such as biomass and coal have inherent variability that causes inconsistent fuel streams/heat output that can limit power plant design and performance. A collaborative, ICTAS-supported research effort between researchers in horticulture, mining engineering, and mechanical engineering is being performed on optimizing fuels. Genetically modified biomass

and biomass/coal-blended fuels are two methods being investigated at Virginia Tech to alter feedstock to produce the desired combustion characteristics. Genetically modified biomass will be produced by Dr. Bingyu Zhao's research group (Horticulture) while coal/biomass-blended fuels will be generated from Dr. Gerald Luttrell's research group (Mining Engineering). Dr. Zhao's group will genetically modify switchgrass to alter its cellulose, hemicellulose, and lignin contents. Dr. Luttrell's group will provide coal/biomass-blended feedstocks in the form of briquettes/pellets. Through their patented process, binding agents and a high-pressure process will be used to manufacture biomass/coal feedstocks with different fractions of coal and biomass. The combustion effectiveness of solid fuels, being measured by Dr. Brian Lattimer's research group (Mechanical Engineering), is a balance between the energy required to convert the solid material into gaseous fuel (heat of decomposition) with the energy produced by the gaseous fuel (heat of combustion). The net heat output as a function of temperature for biomass and coal/biomass blends will be used to rank material performance and provide insight on where to optimize fuels to obtain more consistent fuel production.



Institute for Critical Technology and Applied Science
at Virginia Tech
410 ICTAS, Stanger Street (MC0193)
Blacksburg, VA 24061

U.S. Postage
PAID
Permit No. 28
Blacksburg
VA 24060

Virginia Polytechnic Institute and State University does not discriminate against employees, students, or applicants on the basis of race, color, sex, sexual orientation, disability, age, veteran status, national origin, religion, or political affiliation. Anyone having questions concerning discrimination or accessibility should contact the Office for Equity and Inclusion, (540)231-7500.

ICTAS Connection is published by the Institute for Critical Technology and Applied Science at Virginia Tech. Roop L. Mahajan, Director

Please send comments and address corrections to Melissa Wade, mwade05@vt.edu.

Melissa Wade, editor | Alex Parrish, graphic designer

Sustainable Nanoenabled Consumer Products

continued from page 14

manufacturing, use, and disposal that are extremely difficult to measure given the size of these nanomaterials. Moreover, the transport and reaction of these nanomaterials in the air, water, and soil where exposure can occur with the environment, including with humans, must be understood. Finally, impact factors that translate outputs to human and environmental outcomes are also required.

Amounts of specific nanomaterial outputs, the fate and transport of these materials in the environment and in humans, and the risk of health and environmental effects are unknown for most nanomaterials. These large uncertainties that cross all phases of the life cycles of nanomaterials limit the ability of consumers, scientists and engineers, health officials, and governmental agencies to assess the potential risks versus the benefits of these novel materials. Virginia Tech researchers are investigating each of these areas to bridge the gaps in both scientific understanding and data, given the number of products containing nanomaterials.

The Nano in Society Project

The Nano in Society Project brought together four undergraduate researchers with faculty advisors from the departments of Political Science, History, Apparel, Hous-

ing, and Resource Management, as well as the directors of the Office of Undergraduate Research and the College of Liberal Arts and Human Sciences Undergraduate Research Institute. The four students were: Sarah Golden, Political Science Major, Religious Studies Minor; Albert Jesmer, International Studies Major, Economics Minor; Katherine Williams, English Major, Horticulture and History Minors; and Andrew Wanamaker, Majors in Statistics and Political Science.

The purpose of this project was to assist two ICTAS research thrusts--the Nanoscale Science and Engineering Thrust and the Nano-Bio Interface Thrust--by examining issues of public opinion, media coverage, and policy deliberations in the NCPI (Project on Emerging Nanotechnologies, hosted by Wilson Center in DC). The students devised a set of sample questions that tested attitudes toward nanotechnology, particularly as used in clothing and beverages. After securing approval from Virginia Tech's Institutional Review Board, the students administered this survey to Virginia Tech university students. According to the results, 70 students revealed more positive attitudes toward the use of nanotechnology in everyday products, as compared to the general public surveyed by the Wilson Center. This research project will lead to future collaborations between students in the social and human sciences and researchers in scientific and engineering fields.