B&ESD Newsletter November 2011

Pubs and Products

Chhabra, S. R., Butland, G., Elias, D. A., Chandonia, J.-M., Fok, O.-Y., Juba, T. R., Gorur, A., Allen, S., Leung, C. M., Keller, K. L., Reveco, S., Zane, G. M., Semkiw, E., Prathapam, R., Gold, B., Singer, M., Ouellet, M., Szakal, E. D., Jorgens, D., Price, M. N., Witkowska, H. E., Beller, H. R., Arkin, A. P., Hazen, T. C., Biggin, M. D., Auer, M., Wall, J. D., and J. D. Keasling. 2011. Generalized schemes for high-throughput manipulation of the *Desulfovibrio vulgaris* genome. *Appl. Environ. Microbiol.* 77: 7595-7604.

Department of Energy (DOE) Report to Congress on Climate Change and Federal Hydropower (Section 9505 Report)—summarizing report for DOE concurrence review and submission to Congress expected to be sent from DOE in early FY12.

Ebadian, M., Sowlati, T., Sokhansanj, S., Stumborg, M., and L. Townley-Smith. 2011. A new simulation model for multi-agricultural biomass logistics system in bioenergy production. *Biosyst. Eng.* 110: 280-290.

Garten, C. T., Jr., 2011. Comparison of forest soil carbon dynamics at five sites along a latitudinal gradient. *Geoderma* 167-168: 30-40.

Gu, L., Massman, W. J., Leuning, R., Pallardy, S. G., Meyers, T., Hanson, P. J., Riggs, J. S., Hosman, K. P., and B. Yang. 2012. The fundamental equation of eddy covariance and its application in flux measurements. *Agr. Forest Meteorol.* 152: 135-148.

Guo, W., Bi, X., Lim, C. J., and S. Sokhansanj. 2011. Determination of kinetic parameters of self-ignition wood pellets during storage. Paper presented at the American Institute of Chemical Engineers (AICHE) Conference, October 16th-21st. Minneapolis Convention Center, Minneapolis, MN.

Lam, P. K., Sokhansanj, S., Lim, C. J., Bi, X., and S. Melin. 2011. Energy input and quality of pellets made from steam exploded Douglas Fir (Pseudotsuga menziesii). *Energy Fuels* 25: 1521-1528.

Langholtz, M., Graham, R., Eaton, L., Perlack, R., Hellwinkel, C., and D. G. De La Torre Ugarte. 2011. Price projections of feedstocks for biofuels and biopower in the U.S. *Energ. Policy* Available online. DOI: 10.1016/j.enpol.2011.11.009

Larsson, S. H., Lestander, T. A., Crompton, D., Melin, S., and S. Sokhansanj, 2012. Temperature patterns in large scale wood pellet silo storage. *Appl. Energ.* 92: 322-327.

Lavoie, B., Mayes, M. A., and L. D. McKay. Transport of explosive residue surrogates in saturated porous media. 2011. *Water Air Soil Poll*. Available online. DOI 10.1007/s11270-011-0999-y

Lee, X., Goulden, M. L., Hollinger, D. Y., Barr, A., Black, T. A., Bohrer, G., Bracho, R., Drake, B., Goldstein, A., Gu, L., Katul, G., Kolb, T., Law, B. E., Margolis, H., Meyers, T., Monson, R.,

Munger, W., Oren, R., Paw U, K. T., Richardson, A. D., Schmid, H. P., Staebler, R., Wofsy, S., and L. Zhao. 2011. Observed increase in local cooling effect of deforestation at higher latitudes. *Nature* 479: 384-387.

Li, H., Liu, X., Legros, R., Bi, X. T., Lim, C. J., and S. Sokhansanj. 2012. Torrefaction of sawdust in a fluidized bed reactor. *Bioresource Technol.* 103: 453-458.

Oladosu, G., Kline, K., Martinez, R., and L. Eaton. 2011. Sources of corn for ethanol production in the United States: A review and decomposition analysis of the empirical data. *Biofuel. Bioprod. Bior.* 5: 640-653.

Shrestha, B., Wood, H. C., and S. Sokhansanj. 2011. Microwave dielectric properties of alfalfa leaves from 0.3 to 18 GHz. *IEEE T. Instrum. Meas.* 60: 2926-2933.

Takagi, H., Saeki, T., Oda, T., Saito, M., Valsala, V., Belikov, D., Saito, R., Yoshida, Y., Morino, I., Uchino, O., Andres, R. J., Yokota, T., and S. Maksyutov. 2011. On the benefit of GOSAT observations to the estimation of regional CO2 fluxes. *Scientific Online Letters on the Atmosphere (SOLA)* 7: 161-164.

Zheng, W., Liang, L., and B. Gu. 2012. Mercury reduction and oxidation by reduced natural organic matter in anoxic environments. *Environ. Sci. Technol.* 46: 292-299.

Notable Achievements

Glenn Cada's work on fish-friendly turbines was mentioned in the article, "Hydropower's fish-friendly turbines" by Drew Robb for the website Renewable Energy Focus. Read the article online at http://www.renewableenergyfocus.com/view/19183/hydropowers-fishfriendly-turbines.

On October 11th Shahab Sokhansanj participated in a kick off meeting on logistics modeling of the DOE-funded FDC Enterprises (FDCE) project, "Design and Demonstration of an Advanced Agricultural Feedstock Supply System for Lignocellulosic Bioenergy Production." The modeling effort is targeted at reducing the harvest, staging, and hauling costs associated with three types of harvest and biomass handling machines: (1) a Bale Picking Truck, (2) a Self Loading Trailer, (3) a Self Propelled Large Square Baler (3' x 4' x 8'). The project also includes testing a one step window baling system in terms of target cost reductions of \$13.25 per delivered ton. The analysis efforts will be coordinated with field measurements on demonstration of a mobile/modular grinding system that will enable remote processing of round and square bales in a single grinding step. The model will evaluate the assumptions used in the amount of dust generation and minimal yield losses that will produce feedstock of a quality suitable for refinery requirements in terms of sizing, consistency, and processing characteristics. Learn more about FDCE at http://fdcenterprises.com/home.html.

Yetta Jager conducted a scientific review of "Alternative San Joaquin River Flow Objectives for the Protection of Fish and Wildlife" for the California Environmental Protection Agency (EPA).

During October 23rd-26th the presentation "Torrefaction of BC Softwood" was given at the 61st Canadian Chemical Engineering Conference in London, Ontario, Canada. Coauthors included T. Boyd, H. Kempthorne, G. Lee, S. Sokhansanj, and B. Ghiasi.

During October 31st-November 4th Laura Johnson visited from Indiana University to collaborate with Natalie Griffiths on a research project investigating coupled nutrient cycling in Walker Branch.

On November 1st Jeremy Smith delivered the Keynote Lecture at the International Conference on Computational Physics held in Gatlinburg, TN.

Oak Ridge National Laboratory (ORNL) Water Power Technologies team (Brennan Smith, Boualem Hadjerioua, Vince Neary, Mark Bevelhimer, and Shelaine Hetrick) participated in the Water Power Peer Review (Washington, D.C.) November 1st-3rd. Presentations were given on the Hydropower Advancement Project (Smith), Effects on Aquatic Organisms (Acoustics and Toxicity) (Bevelhimer), Non-Powered Dams Resource Assessment (Hadjerioua), Climate Change Assessment (Mike Sale), and Conventional Hydropower Environmental Hurdles: Instream Flow (Bevelhimer). The ORNL team provided input for presentations on marine and hydrokinetic (MHK) Reference Models, MHK Environmental electric and magnetic fields (EMF), Water Use Optimization, Basin Scale Opportunity Assessment and Quantifying Full Value of the Hydro in Transmission Grid activities.

On November 2nd Virginia Dale, Allen McBride and Bruce Bunting had a conference call with Jeremey Alcorn of the Logistics Management Institute (LMI) about the work on sustainability of biofuels that LMI is conducting for the Defense Logistics Agency (DLA) related to the Defense Production Act. This topic builds from the Final National Defense Authorization Act (NDAA) FY10 Section 334 Report as adopted by the Department of Defense (DoD) and submitted to Congress that is titled "DoD Report: Opportunities for DoD use of Alternative and Renewable Fuels."

Also on November 2nd Keith Kline, Gangsheng Wang, and Michael Wang (Argonne National Laboratory [ANL]) contributed to the 8th webinar for International Organization for Standardization (ISO) PC 248 (Bioenergy Sustainability) Working Group 2 – Greenhouse Gas Emission Methods – discussing a set of selected issues and developing agreement on revised language for the corresponding chapter of the report.

On November 2nd Shahab Sokhansanj participated in a kick-off meeting on logistics modeling of the DOE-funded Genera project "Development of a Bulk-Format System to Harvest, Handle, Store, and Deliver High-Tonnage Low-Moisture Switchgrass Feedstock." The modeling efforts will focus on developing simulations of the base baling and the proposed bulk flow options. The Integrated Biomass Supply and Logistics Model (IBSAL) will model the complete cycle of baling using the data input from the project. For the bulk flow, data obtained from experiments in the lab and in the field and the available data and experiences on similar systems elsewhere (handling and processing grasses for transport and feeding) will be used. IBSAL will analyze switchgrass production, options for collecting and harvesting, sizing and organizing in-field storage depots, preprocessing, and eventually optimum management strategies for just-in-time delivery of feedstock to the DuPont Cellulosic Ethanol plant in Vonore, TN.

During November 2nd-4th Tom Wilbanks was a speaker and participant in an international meeting at the National Center for Atmospheric Research (NCAR) on The Development of Socioeconomic Pathways for Climate Research.

Dale Kaiser attended The National Climate Assessment (NCA) Climate Science Working Group Forum on "Trends and causes of observed changes in heat waves, cold waves, floods and drought," at the National Climatic Data Center in Asheville, NC. He chaired the session on heat

and cold waves and is coordinating lead author on the heat and cold waves section of a paper to be submitted to the *Bulletin of the American Meteorological Society*. The paper will reflect the scientific results presented in the forum and our current understanding of trends and causes of heat and cold waves in the United States. Also at the meeting, Dale gave a presentation on "Changes in False Spring-Related Cold Waves over the Southeastern United States."

On November 5th a symposium inspired by the work of Pat Mulholland titled "Global change effects on aquatic ecosystems: insights into controls on ecosystem functions and implications for their protection, conservation, and restoration" was held at the American Museum of Science and Energy in Oak Ridge, TN. Eleven talks throughout the day highlighted Pat's contributions to aquatic ecology and biogeochemistry, with topics ranging from stream carbon and nutrient dynamics, river restoration, and science policy. Over 45 of Pat's colleagues traveled from across the country to participate in this memorable event.

Jonathan Mielenz presented ORNL research results to the Society for Industrial Microbiology's Recent Advances in Fermentation Technology IX meeting in Florida. The title of the presentation was "Better bugs meet better biomass: Potential of synergies of superior bioconversion microorganisms and improves biomass sources," describing the BESC-funded ORNL research using an improved yeast from Mascoma combined with Noble Foundation transgenic switchgrass.

On November 7th-8th Stephen Sebestyen (from the United States Forest Service [USFS] Northern Research Station) met with ORNL collaborators to discuss the technical and scientific aspects of water research on the Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) project.

Several members of the Biosciences Division (BSD) presented lectures as part of a four-part course associated with the Oak Ridge Institute for Continued Learning (ORICL) entitled "The Molecules of Life" and led by Jeremy Smith. The lectures were held at the Oak Ridge campus of Roane State Community College. Jerry Parks gave a lecture on November 8th entitled "Mercury in the Environment: What are Bacteria Doing About It?" Loukas Petridis also presented a lecture, "Biofuels. Why plants are recalcitrant to letting themselves be turned into "grassoline" and what ORNL supercomputers doing about it." Jeremy C. Smith presented "The Molecules of Life. We will look at how the molecules of life function, and how ORNL supercomputers and neutron scattering facilities investigate this to design new drugs and to overcome barriers to biofuel production" on November 29th.

On November 9th Jeremy Smith gave the Plenary Lecture at the International Symposium on Clusters and Nanostructures (Energy, Environment and Health) held in Richmond, VA.

For DOE's Office of Science and during November 9th-10th, Tom Wilbanks organized and conducted an expert workshop for the U.S. NCA on Climate Change and Infrastructure, Urban Systems, and Vulnerabilities in Washington, DC.

During November 9th-11th Melanie Mayes presented her poster, Controls on layer formation of natural organic carbon on soils, at the ORNL Neutron Scattering User Meeting. Coauthors include S. Jagadamma, H. Ambaye, L. Petridis, and V. Lauter.

On November 11th Jeremy Smith presented a lecture at the Symposium on Neutrons and Simulation held at the Spallation Neutron Source (SNS) at ORNL.

Dale Kaiser took part in the National Oceanic and Atmospheric Administration (NOAA)-Roshydromet Bilateral Program's "Workshop on Improved Quality of Data and Data Exchange for Climate Research and Analysis" at the National Climatic Data Center, Asheville, NC. Roshydromet is the Hydrometeorological Service of Russia. Dale worked with Russian colleagues from the All-Russian Institute of Hydrometeorological Information - World Data Center (RIHMI-WDC) in arranging for continued acquisition, quality assurance, documentation, and distribution (through the Carbon Dioxide Information Analysis Center [CDIAC] website) of key Russian surface-meteorological datasets.

Donna Kridelbaugh received a travel subsidy to serve as a scientific judge at the Annual Biomedical Research Conference for Minority Students (ABRCMS), held November 9th-12th in St. Louis, MO. The interdisciplinary conference for biomedical and behavioral science students, including mathematics, is supported by a range of science disciplinary societies and managed by the American Society for Microbiology (ASM) Education Department. A main objective of the meeting is "increasing diversity to improve global scientific competitiveness" with a format designed to encourage minority students to seek advanced training in graduate programs or research internships. Next year's conference is scheduled for November 7th-12th, 2012, in San Jose, CA. For more information on attending or judging the conference, visit: http://www.abrcms.org.

Chris Lenhardt participated in a telecom of the Earth Science Information Partners (ESIP) Federation Executive Committee on November 10th.

Oak Ridge National Laboratory's Director of Energy Efficiency and Electricity Technologies Program, Tom King, and the Water Power Technologies Program Manager, Brennan Smith, visited with Jose Zayas, the new Wind and Water Program Manager for DOE in Washington, D.C., on November 10th.

Baohua Gu recently participated in proposal reviews for the Phase I Small Business Innovation Research (SBIR) supported by the U.S. DOE.

On November 10th Shahab Sokhansanj travelled to Forest Concepts Inc. in Auburn, WA, to conduct a day of discussion on size reduction and dryer design with Jim Dooley and his engineering science staff. Forest Concepts (www.forestconcepts.com) focuses on R&D related to biomass and bioenergy. The company also has a longer-term contract to provide specialty packages of feedstocks for various applications. Forest Concepts receives competitive funding from DOE, the United States Department of Agriculture (USDA), and other government and private industry in support of its research. Discussion topics on November 10th were limited to the Company's latest effort in developing size reduction systems to produce low cost uniform particles with closely controlled sizes "crumbles," a new pilot scale biomass dryer, and biomass fractionation equipment. These discussions were accompanied by a visit to the Company's lab and workshops.

Melanie Mayes received the Young Alumni Award from the Chair of the University of Tennessee Department of Earth and Planetary Sciences, Larry McKay, on November 10th. Melanie received the award for her "success in research and strong support for the department, through student mentoring and collaborative research projects and grants."

During November 10th-11th Virginia Dale visited Michigan Technological University as a Distinguished Ecologist lecturer in the School of Forest Resources and Environmental Science and gave a lecture on "Steps towards Bioenergy Sustainability."

On November 11th Liyuan Liang presented an invited talk at Northwestern University on ORNL mercury research entitled "Mechanisms controlling mercury speciation in a contaminated environment: role of naturally dissolved organic matter."

On November 11th and 12th Natalie Griffiths participated in the Meta-Analysis & Synthesis of Leaf Decomposition in the Streams working group meeting at the Coweeta Hydrologic Laboratory in Otto, NC.

During November 13th-16th Mike Hilliard presented at the Annual Meeting of the Institute for Management Science and Operations Research (INFORMS) in Charlotte, NC, on the Biomass Location for Optimal Sustainability Model (BLOSM) --Balancing Profit and Water Quality in a Watershed. His presentation used data from the watershed surrounding a cellulosic ethanol refinery in Tennessee. An optimization model paired with results from a water quality model demonstrates that planting switchgrass in the right locations can improve nitrogen, phosphorus and sediment levels with a moderate impact on revenue. A web-based interface communicates the results and can be seen at

 $\frac{https://informs.emeetingsonline.com/emeetings/formbuilder/clustersessiondtl.asp?csnno=15781\&mmno=206\&ppnno=57555.$

During November 13th-17th Trent Jett, Teresa Mathews, Carrie Miller, Mark Peterson, Kelly Roy, and John Smith conducted a field study on the dynamics of mercury and tin in three small streams on the Savannah River Site near Aiken, SC. The study is a collaborative effort with staff from the Savannah River National Laboratory and the Savannah River Ecology Laboratory. Sediment, water, fish, and invertebrate samples were collected and will be analyzed for tin, mercury, and other metals. The study is funded by the Department of Energy (DOE) Office of Technology Innovations & Development (EM-30) Groundwater & Soil Remediation Program (EM-32).

During November 15th-16th Virginia Dale participated in a Southeastern Partnership for Integrated Biomass Supply Systems (IBSS) Inaugural charrette meeting in Knoxville to kickoff plans for this United States Department of Agriculture (USDA)-funded project that involve several universities and private companies from across the region.

Shih-Chieh Kao participated in the National Water Resources Association (NWRA) Annual Conference in Tucson, AZ, during November 15th-17th. Shih-Chieh Kao aided in conference dissemination of information about the DOE Water Program and ORNL Water Power Technologies research through involvement in discussion groups and networking.

Tim Hendrick made a presentation entitled "Invest in Energy Efficiency? Homeowner Decision Making and Major Energy Retrofits" at the 2011 Behavior, Energy, and Climate Change conference in Washington, D.C.

Bob Perlack was invited to present the U.S. Billion-Ton Update to the Laboratory Energy Research & Development Working Group (LERDWG) on November 16th in Washington, D.C. Virginia Dale talked about the recent National Research Council (NRC) report "Potential Economic and Environmental Effects of U.S. Biofuel Policy."

On November 17th Virginia Dale gave a plenary talk on "Steps towards Bioenergy Sustainability" at the National Science Foundation Emerging Frontiers in Research Innovation, Resilient and Sustainable Infrastructures Program (NSF-EFRI RESIN) Workshop in Champaign, IL. Learn

more about the NSF-EFRI-RESIN workshop at http://ict.illinois.edu/conferences/RESINworkshop2011/.

Bo Saulsbury gave the presentation "Fueleconomy.gov: NewFeatures and Tools" at the 2011 Clean Cities Coordinator Regional Peer Exchange in Dallas, TX, on November 17th.

Shahab Sokhansanj contributed to the development of the Biomass Research and Development Initiative (BRDI) research proposal "Sustainable Production System for Cellulosic Fuels and Biobased Products Using Mixed Alcohol and Pyrolysis Conversion Methods." Texas A&M AgriLife Research (Lloyd Ted Wilson) leads the proposal with Mississippi State University, Washington State University, and Oak Ridge National Lab. The industrial partners are Terrabon, TX, Piedmont BioProducts, VA, and REPREVE Renewables, GA. The total project cost is \$8,743,388 over 4 years. The proposed research addresses major barriers to the expansion of the cellulosic bioenergy industry through achievement of the following overall objectives:

- 1) Develop sustainable extended-season systems for the production, harvest, storage, and delivery of biofeedstocks
- 2) Improve process efficiencies for the mixed-alcohol and pyrolysis conversion methods leading to economically competitive commercial-scale production
- 3) Evaluate the economic, social, and environmental impact of targeted bioenergy production systems via integrated life cycle analysis and multi-model based process optimization through the supply chain from feedstock production through product distribution Long-term impacts of the proposed project include greater expansion and viability of the bioenergy industry, improved environmental and economic performance, improved rural prosperity and development, reduced food market effects, and greater energy independence.

Amy Wolfe participated in a panel called "Come Hell or High Water: Legacies and Landmarks in the Cultures of Energy" at the American Anthropological Annual Meeting in Montreal, Canada, on November 17th.

Giri Palanisamy was highlighted in the October issue of the Climate Change Science Institute (CCSI) Newsletter. Learn more about the CCSI at www.climatechangescience.ornl.gov.

On November 18^{th} Rebecca Efroymson presented "Environmental Scientists: Who We Are and What We Do" to 3^{rd} , 4^{th} , 5^{th} graders at Haw Creek Elementary School, Asheville, NC.

The beta version of the new FLUXNET website is available for viewing. The website is built with the Drupal content management system on top of a PostgreSQL database and can be seen at http://fluxnet-dev.ornl.gov.

On November 21st Shujiang Kang, Mac Post, Keith Kline and other staff discussed the work plan for developing a prototype global bioenergy crop model in coordination with the Global Sustainable Bioenergy (GSB) project. Initial work, supported by in-house program development funds, will focus on calibrations for switchgrass.

On November 22nd Maggie Davis and Keith Kline contributed to the 11th webinar of ISO PC 248 (Bioenergy Sustainability) Working Group (WG) 4 – Indirect Effects – that focused on the final two sections of the WG4 draft report on mitigation and synthesis of state of science. ORNL WG members also contributed over 40 citations (approximately 30% of all citations submitted) to the annotated bibliography that forms an integral part of the WG4 report.

On November 29th the presentation "Improving analysis of environmental effects of bioenergy feedstock production: Identifying issues and endpoints" was given by Rebecca Efroymson at the Biofuels and the Environment Workshop on Environmental Assessment Endpoints for Feedstock Production in Washington, D.C. Coauthors included P. B. Woodbury and E. DeLucia.

On November 29th Yetta Jager contributed to a proposal for a special session at the 2012 Ecological Society Meeting in Portland, entitled "A Debate on the Sustainability of Biomass Production for Energy." Debaters were identified and invited to represent two "sides" of three issues: 1) effects on biodiversity, 2) effects on habitat, and 3) effects on invasive species. Other organizers include Caroline Ridley (EPA), Zakiya Leggett (Weyerhaueser), and Chris Clark (EPA).

On November 29th Alex Johs presented recently published neutron scattering results from the Mercury Science Focus Area (SFA) at a visit by Sharlene Weatherwax (Biological and Environmental Research [BER] Associate Director of Science) to the SNS and the High-Flux Isotope Reactor (HFIR) hosted by Kelly Beierschmitt, Paul Langan (Neutron Sciences Directorate) and Martin Keller.

For DOE's Office of Science Tom Wilbanks organized and conducted an expert workshop for the U.S. NCA on Climate Change and Energy Supply and Use in Washington, D.C., November 29th-30th.

During November 29th-December 1st Rebecca Efroymson, Yetta Jager and Virginia Dale participated in a workshop on EPA conceptual models that diagram activities and potential impacts of biofuel feedstock production. These conceptual models were first developed for EPA's Biofuels and the Environment: First Triennial Report to Congress. In addition to providing written reviews of the conceptual models, Virginia gave a brief presentation and chaired a panel discussion. Yetta presented her review of conceptual model pathways as they influence water as an endpoint.

The poster "Geochemical controls on sorption and transport of nitroaromatic compounds (Trinitrotoluene [TNT] and Cyclonite [RDX]) in soils from Massachusetts Military Range" was presented at the Partners in Environmental Technology Technical Symposium and Workshop, November 29th- December 1st in Washington, D.C. Coauthors were M. A. Mayes, P. Sharma, and G. Tang.

The poster "Modeling coupled dissolution, solute, and particle transport of explosive residue in saturated porous media" was also presented at the Partners in Environmental Technology Technical Symposium and Workshop, November 29th- December 1st. Coauthors were G. Tang, M. A. Mayes, P. Sharma, B. Lavoie, and L. D. McKay.

On November 30th Shahab Sokhansanj participated in a kick-off meeting on logistics modeling of the DOE-funded AGCO project, "Integration of advanced logistical systems and focused bioenergy harvesting technologies to supply crop residues and herbaceous energy crops in a densified large square bale format." The modeling efforts will focus on developing simulations for all stages of large square and round bales supply chains, beginning with field harvest and continuing through storage and preprocessing, and quality changes during storage. The model will evaluate biomass of varying moisture and compositional characteristics, and determine how bale variation influences supply chain efficiency and biomass quality following storage.

BESD New Arrivals

Jiafu Mao reported to work in November, working as an Earth System Modeling Scientist with Mac Post in the Environmental Sciences Division's (ESD) Ecosystem Science group.

Xiaoying Shi also reported to work in November, working as an Earth System Modeling Scientist with Mac Post in the ESD Ecosystem Science group.