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Biological and Environmental Research

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Annual Report FY 2009

Oak Ridge National Laboratory (ORNL) conducts basic and applied research and development to create scientific knowledge and technological solutions that strengthen the nation's leadership in key areas of science; increase the availability of clean, abundant energy; restore and protect the environment; and contribute to national security.

Foreword

Martin Keller
Associate Laboratory Director
Biological and Environmental Sciences
Oak Ridge National Laboratory

Fiscal year 2009 was a year filled with change and amazing progress for the Biological and Environmental Sciences (BES) Directorate. Between Dr. Reinhold Mann's departure in November 2008 until my arrival in June 2009, Dr. Gary Jacobs served as our interim Associate Laboratory Director. I know I speak for everyone in BES and across ORNL when I thank Gary for all his hard work and the invaluable support he provided during this transition period.

A collaborative and interdisciplinary approach to biological research—a New Biology—is recommended in *A New Biology for the 21st Century*, a report recently published by the national academies. Prepared by a committee of representatives from the National Academy of Sciences, the National Academy of Engineering, the Institute of Medicine, and the National Research Council, the report examines the current state of biological research and recommends how the United States might best capitalize on recent technological and scientific advances. Several multidisciplinary projects of key societal importance are suggested that include adaptation of food plants to local growing conditions, ecosystem monitoring and restoration, combining crop research and microbial engineering to make biofuels a viable alternative to fossil fuels, and personalized medicine to improve health care. This new approach requires greater integration within areas of biological research, closer collaboration with scientists of different disciplines, and increased leveraging of resources across federal, private, and academic sectors. Although our directorate is already actively engaged in many of these recommendations and suggested multidisciplinary projects, we, and all of ORNL, continue to expand our cross-disciplinary approach among our many areas of research in an effort to provide solutions to the world's major technological challenges.

In this spirit, we continued to support cross-cutting research teams and projects at ORNL to further advance science and contribute to the missions of the Department of Energy. The multidisciplinary BioEnergy Science Center (BESC) has already made substantial progress toward the goal of overcoming biomass recalcitrance. Using an integrated approach to solving the challenge of producing biofuel from cellulosic materials, the center will not only provide the scientific basis for affordable and sustainable biofuel but will also advance our understanding in areas of fundamental biological science. After 2 years of operation, BESC has already achieved scientific breakthroughs that demonstrate proof of concept and has accelerated the initial 5-year timeline by more than 1 year. The center has also managed to integrate its scientific activities and demonstrate considerable synergy beyond individual research projects. BESC researchers have published over 100 scientific articles, 60% of which represent multi-institution collaborations both within BESC and throughout the scientific community.

ORNL recently initiated a cross-cutting Climate Change Science Institute (CCSI) with the goal of further aligning climate change science across the Laboratory. Under the leadership of Dr. Jim

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Hack, staff from various directorates will focus their attention on four thrust areas: Carbon Cycle and Ecosystem Science; Earth System Modeling; Climate Data Integration, Dissemination, and Informatics; and Climate Impacts, Vulnerabilities, and Adaptation Science. I look forward to their future contributions in this area of research.

ORNL also established the Center for BioEnergy Sustainability (CBES) to bring together the unique skills and technical expertise of the ORNL staff in addressing sustainability issues of national and global concern related to environmental impact and biomass production, and the conversion of biomass to biofuels and bio-based products. The mission of CBES is to better understand the sustainability (environmental, economic, and social) of current and future bioenergy production and distribution; to identify approaches that enhance bioenergy sustainability; and to serve as an independent source of the highest quality data and analyses available to bioenergy stakeholders and decision-makers. The CBES provides opportunities for ORNL scientists and other stakeholders to work collaboratively and develop strategies that best address these challenges.

Another area of focus this year was the implementation of the new BER Office of Science funding models. Scientific projects will now be divided into Science Focus Areas (SFA). We have established SFAs in Fundamental Science, Bioenergy, Climate Change Research, Subsurface Science, Ethical, Legal and Societal Implications, Low-Dose Radiation, and Radiochemical Imaging. These SFAs will provide us additional opportunities to create research programs spanning various scientific disciplines.

Our Directorate, consisting of the Biosciences Division and the Environmental Sciences Division, covers a wide span of business lines that includes bioenergy, climate and environmental change, stewardship science, data and bionformatics, biomedical science, and sensor technology. Our research involves scientists from across ORNL as well as other institutions as we move more and more toward a multidisciplinary culture.

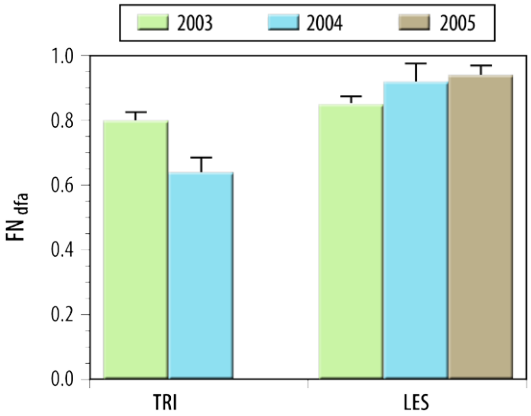
I hope you will enjoy reading about our recent research and the inspiring work being performed by our staff as we continue to collaborate with other scientists across the nation and around the world in an effort to provide viable and timely solutions to the serious scientific and technological challenges facing our world today.

Research Highlights

CLIMATE CHANGE

Nitrogen fixation controls old-field ecosystem response in a multi-factor climate change experiment

Understanding the effects of complex environmental interactions and dynamic changes on microbial community composition and nitrogen fixation as a result of climate change requires multi-species studies. In this investigation, ORNL scientists measured nitrogen fixation and ecosystem response in an old field under varying combinations of elevated or ambient CO_2 concentrations, increased or ambient temperature, and decreased or ambient soil moisture.



Mean (±SE) fraction of tissue N derived from atmospheric N_2 fixation (FN_{dfa}) by Trifolium *(TRI) and* Lespedeza *(LES) in 2003, 2004, and 2005. Mean values are based on 23 or 24 measurements.*

Although treatment results varied from year to year, the scientists found that symbiotic nitrogen fixation by legumes was a primary controller in changing old-field species composition during the 3-year study and annually contributed 44–51% to the standing nitrogen stock in aboveground old-field biomass. The biomass of *Lespedeza*, a key legume that bears nitrogen-fixing bacteria on its roots which increase soil nitrogen content, grew faster than the other plant species, including *Trifolium*, thus increasing its importance to total aboveground biomass regardless of manipulated environmental factors.

Changes in species composition over time in the old-field community were found to have a more significant impact on the nitrogen cycle than the response of individual species to the experimental treatments. Although seemingly unresponsive to the environmental manipulations, symbiotic nitrogen fixation was a primary controller in changing old-field species composition over the course of the experiment. Such effects of climate change resulting from complex interactions between the environment and ecosystem response are overlooked in single-species experiments.

C. T. Garten, Jr., A. T. Classen, R. J. Norby, D. J. Brice, J. F. Weltzin, and L. Souza. "Role of N_2-fixation in constructed old-field communities under different regimes of [CO_2], temperature, and water availability," **Ecosystems** 11: 125–137 (2008).

CO_2 enrichment increases carbon and nitrogen input from fine roots in a deciduous forest

The production of fine roots (each less than 2 mm in diameter) is expected to increase under elevated concentrations of atmospheric CO_2, especially in nitrogen-limited forests where increased belowground carbon allocation may facilitate nitrogen acquisition. Greater fine-root production under elevated concentrations of CO_2 may drive changes in soil carbon storage and nitrogen cycling because fine roots turn over quickly in forested ecosystems. However, the rate at which carbon and

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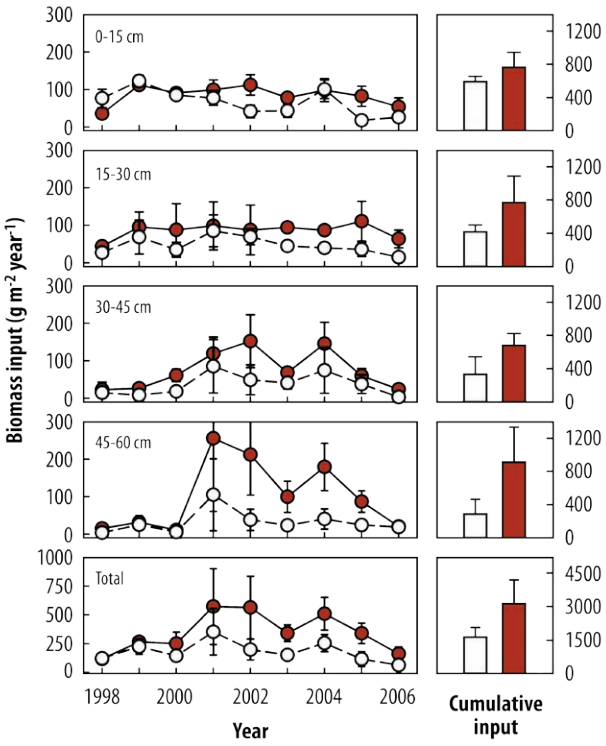
nitrogen are re-mineralized from fine-root detritus will depend on root population turnover and chemistry, as well as on the soil depth at which the roots are produced.

Scientists at ORNL assessed the effects of elevated concentrations of CO_2 on the production and mortality of short-lived fine-root populations at several soil depths. This research was part of the ORNL Free-Air CO_2-Enrichment (FACE) experiment being conducted at a sweetgum (*Liquidambar styraciflua* L.) plantation in eastern Tennessee where the trees were exposed to ambient or elevated atmospheric CO_2 concentrations since 1998. The scientists found that CO_2 enrichment doubled fine-root production and mortality over 9 years, providing inputs to the soil system of 681 g/m^2 of additional carbon and 9 g/m^2 of additional nitrogen. However, no effect was observed on fine-root tissue density or nitrogen concentration within a given diameter class. At least half of root inputs were below a soil depth of 30 cm, where the microbial mineralization of carbon and nitrogen from fine-root detritus may be limited by soil temperature, oxygen availability, or moisture.



Average annual and cumulative root biomass inputs were greater under elevated concentrations of CO_2, especially at depth in the soil.

Quantification of the effects of elevated CO_2 on fine-root detritus and its subsequent decomposition, especially at depth in the soil, will provide critical information needed for predicting processes such as long-term soil carbon storage and nitrogen cycling in response to environmental change.

C. M. Iversen, R. J. Norby, and J. Ledford. "CO_2 enrichment increases carbon and nitrogen input from fine roots in a deciduous forest," **New Phytologist** 179: 837–847 (2008).

CDIAC estimates of CO_2 emission from fossil-fuel use and cement production

The Carbon Dioxide Information Analysis Center (CDIAC) at Oak Ridge National Laboratory, which includes the World Data Center for Atmospheric Trace Gases, has served as the primary climate-change data and information analysis center of the U.S. Department of Energy since 1982.

Each year CDIAC quantifies the release of carbon from fossil-fuel combustion and cement production at global, regional, and national spatial scales. The emissions time series estimates are based largely on annual energy production and use statistics published by the United Nations and cement production data from the U.S. Geological Survey. The latest updates estimate the global release from fossil-fuel consumption and cement production to be 8.23 billion tons of carbon for 2006,

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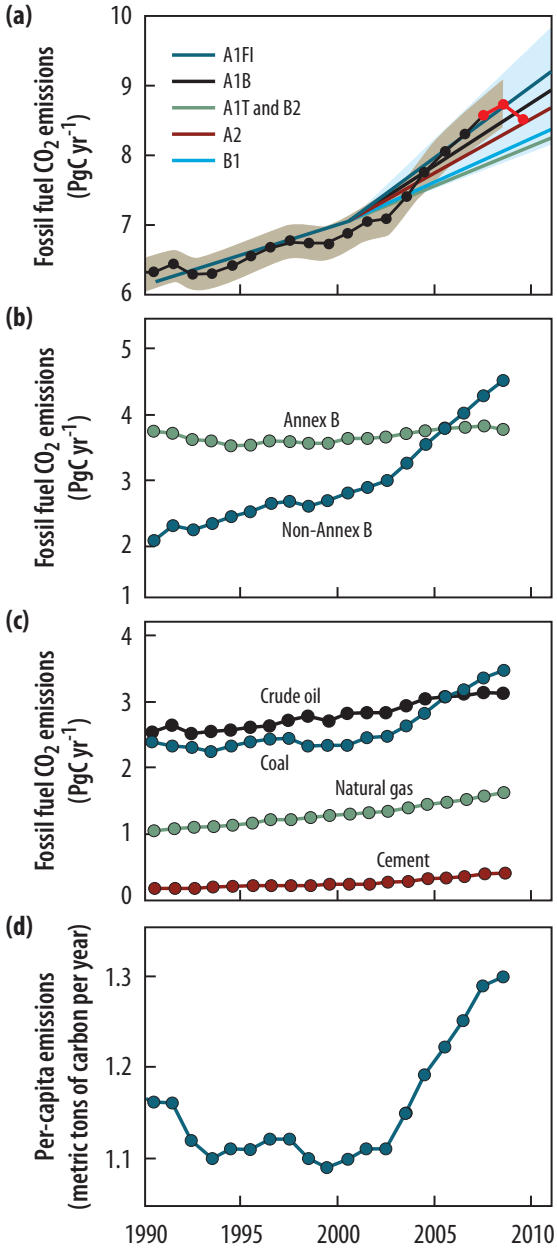
an all-time high. CDIAC estimates that since the year 1751 approximately 329 billion tons of carbon has been emitted to the atmosphere from fossil-fuel combustion and cement production, with half the release occurring since the 1970s. Preliminary estimates indicate that high growth rates are continuing and that global emissions for 2008 have reached 8.67 billion tons of carbon.

According to the latest updates, two countries—the People's Republic of China (PRC) and the United States—each annually emit more than 1.5 billion tons of carbon. The United States has long been the world's largest consumer of fossil fuels, accounting for ~40% of the world's fossil-fuel carbon emissions in 1950. According to the latest data, China surpassed the United States as the world's largest fossil-fuel-emitting nation in 2006, a result of remarkable recent economic growth (e.g., a 79% increase in Chinese fossil-fuel carbon releases from 2000 to 2006). According to the 2006 numbers, U.S. and Chinese emissions are three to four times higher than the next largest emitting nations—Russia (427 million tons carbon), India (412), and Japan (353). Regionally, the developed countries of Europe and North America show modest increases in fossil-fuel carbon emissions recently, while emissions from Africa, South America, and especially Asia continue to grow.

For more information and detail, please visit the CDIAC web site at http://cdiac.ornl.gov/trends/emis/overview.html

T. A. Boden, G. Marland, and R. J. Andres. **Global, Regional, and National Fossil-Fuel CO_2 Emissions**, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tenn., 2009, DOI: 10.3334/CDIAC/00001.

C. Le Quéré, M. R. Raupach, J. G. Canadell, and G. Marland. "Trends in the sources and sinks of carbon dioxide," **Nature Geoscience** 2, 831–836 (2009), DOI: 10.1038/ngeo689.



Fossil-fuel CO_2 emissions since 1990. Panel (a)—calculated global fossil-fuel emissions (black dotted line); Panel (b)—emissions from Annex B countries (mostly developed countries) in green and non-Annex B countries (mostly developing countries) in blue; Panel (c)—global emission broken down by major fuel group and from cement production; Panel (d)—global per capita emissions. Panel (a) also shows the projections, averaged by scenario family, from the IPCC Special Report on Emissions Scenarios. The gray shading is the uncertainty in the emissions estimates, and the blue shading covers all CO_2 emissions scenarios used to project climate by the IPCC Fourth Assessment Report. The red dots are the projected emissions for 2009.

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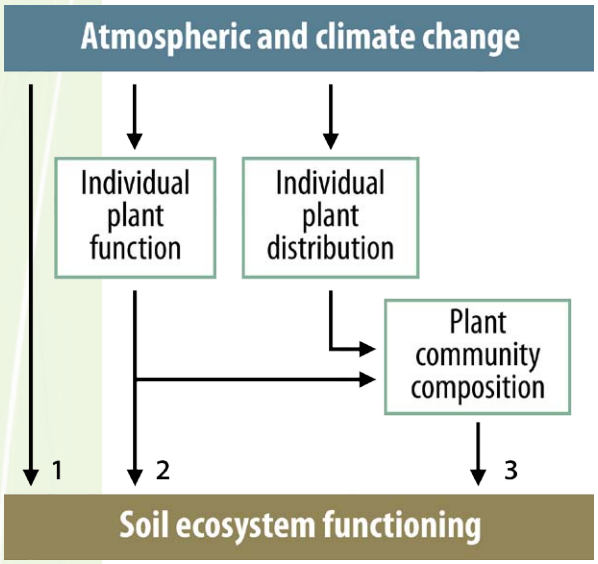
Ecosystem response to atmospheric and climate change

Terrestrial ecosystem responses to atmospheric and climate change—primarily elevated levels of greenhouse gases, such as CO_2, and increased warming of the earth's surface from the greenhouse effect—depend on the dynamics of soil ecosystems, which can respond both directly and indirectly to climate change. To better understand how climate change may alter soil ecosystem functioning, scientists at ORNL investigated old-field plant community and soil ecosystem responses to the combined effects of elevated concentrations of CO_2, warming, and precipitation and the single effects of exposure to any one of these treatments. In the Old-field Climate Change and Atmospheric Manipulation (OCCAM) experiment, they collected soils at the plot level (plant community soils) and beneath dominant plant species (plant-specific soils). Microbial enzyme activities and soil nematodes were used as indicators of soil ecosystem functioning.



Their study resulted in two major findings.

- Although some interactions were observed, water, relative to increases in CO_2 concentration and warming, had the largest impact on plant community composition, soil enzyme activity, and soil nematodes. Multiple climate change factors can interact to shape ecosystems, but the ORNL scientists determined that those interactions were largely driven by changes in water inputs from precipitation.
- Indirect effects of climate change, via changes in plant communities, had a significant impact on soil ecosystem functioning. Climate change effects on enzyme activities, soil nematode abundance, and community structure strongly differed not only between plant community soils and plant-specific soils but also within plant-specific soils.

These results indicate that accurate assessments of climate change impacts on soil ecosystem functioning require incorporating the concurrent changes in plant function and plant community composition. Climate change–induced shifts in plant community composition will likely modify or counteract the direct impact of atmospheric and climatic change on soil ecosystem functioning. Hence, these indirect effects should be taken into account when predicting the extent to which global change will alter the functioning of soil ecosystems.

P. Kardol, M. A. Cregger, C. E. Campany, and A. T. Classen. "Soil ecosystem functioning under climate change: plant species and community effects," **Ecology**, in press.

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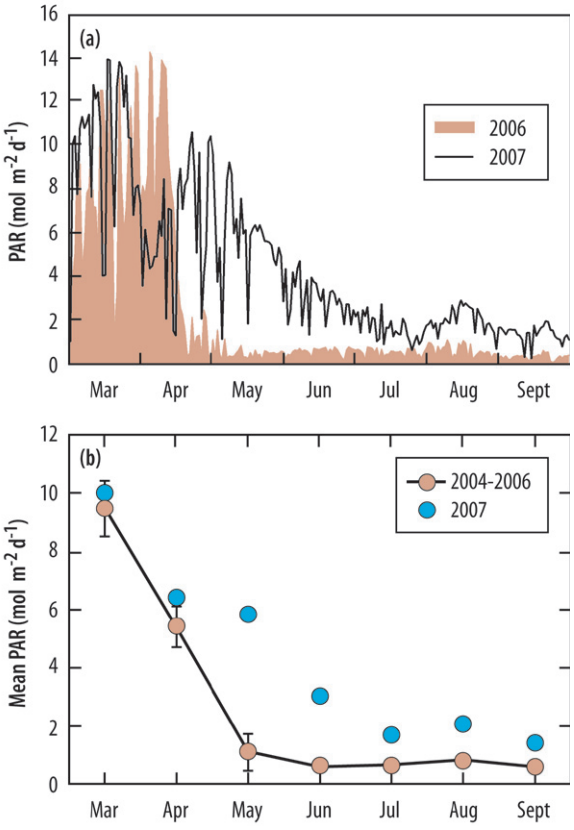
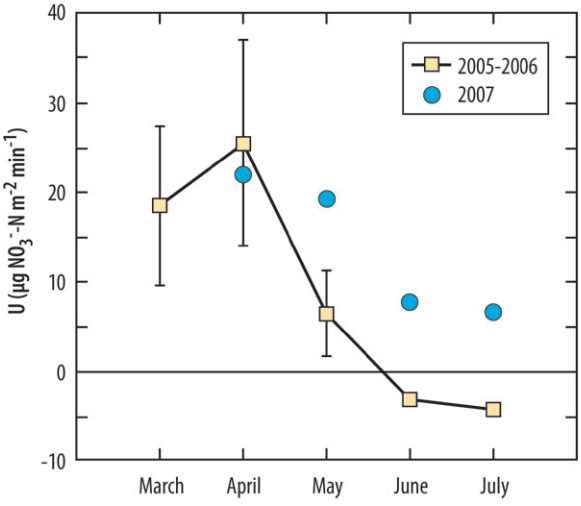
The 2007 spring freeze: unexpected effects of climate change on stream ecosystem

Extreme weather events, such as the spring freeze in 2007 in the eastern United States, are becoming more frequently associated with climate change. The effects of this freeze event on Walker Branch, a well-studied stream ecosystem in eastern Tennessee, were studied by ORNL scientists. Their findings show that changes in forest vegetation dynamics, or phenology, and in canopy structure can have dramatic effects on stream productivity at multiple trophic levels (organism nutrition and feeding habits) and on nutrient cycling as a result of the tight coupling of forest and stream ecosystems.

The 2007 freeze killed newly grown leaf tissues in the forest canopy, dramatically increasing the amount of light reaching the stream. Light levels at the stream surface were considerably higher than those typically observed during the late spring and summer months as a result of the incomplete recovery of the canopy leaf area. A cascade of ecological effects in the stream ensued, beginning with rates of gross primary production (GPP) that were two to three times higher than normal for that time of year. Higher rates of stream GPP in turn led to higher rates of nitrate uptake by the autotrophic community—green plants that use photosynthesis to make complex nutritive organic compounds from simple inorganic sources—and lower nitrate concentrations in the stream water. High GPP rates also resulted in higher growth rates of the snail *Elimia clavaeformis*, a dominant herbivore. Typically, during the summer months, net nitrate uptake and snail growth rates are zero to negative, but in 2007 uptake and growth were maintained at moderate levels.



Daily GPP in Walker Branch from March through September 2007 and mean monthly values of daily stream GPP for March through September 2004 to 2006



Mean monthly rates of net nitrate uptake (U) in Walker Branch for March through July 2005–2006 and in 2007

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These results demonstrate that extreme weather conditions and unpredictable combinations of weather patterns can induce changes in forest canopy structure and phenology that could have significant effects on stream ecosystems in the future.

P. J. Mulholland, B. J. Roberts, W. R. Hill, and J. G. Smith. "Stream ecosystem responses to the 2007 spring freeze in the southeastern United States: unexpected effects of climate change," **Global Change Biology** 15: 1767–1776 (2009), DOI: 10.1111/j.1365–2486.2009.01864.x.

Effects of CO_2 enrichment on forest soil microbial processes and communities

Increased growth of vegetation and enhanced storage of soil carbon under elevated concentrations of CO_2 have been demonstrated in a number of experiments. However, the ability of ecosystems, either above or below the ground, to maintain increased carbon storage depends upon the responses of soil processes to climate change, such as those that control nitrogen mineralization—the decomposition of chemical compounds in organic matter into nitrogen forms that plants can take up and use for new growth. These soil processes are mediated by microbial communities whose activity and structure may also respond to increasing atmospheric CO_2.

Researchers in ORNL's Biosciences and Environmental Sciences divisions and the University of Tennessee's Department of Ecology and Evolutionary Biology took advantage of a long-term, 10-year CO_2 enrichment experiment in a sweetgum tree plantation located in the southeastern United States to test this hypothesis: Observed increases in root production in plots with elevated CO_2, relative to the root mass in ambient CO_2 plots, would alter microbial community structure, increase microbial activity, and boost cycling of soil nutrients needed for plant growth.

The researchers found that elevated CO_2 had no detectable effect on (1) microbial community structure, determined by using 16S rRNA gene clone libraries; (2) microbial activity, measured with extracellular enzyme activity; or (3) potential rates of soil nitrogen mineralization and nitrification—conversion by specialized bacteria of ammonia to nitrites (NO_2^-) and then nitrates (NO_3^-). These results are similar to findings at other forested Free-Air CO_2-Enrichment (FACE) sites. However, differences are very difficult to detect in soil systems due to the complexity and heterogeneity of the soil itself. Further technology development and studies that allow more replicates and more precise sampling are required and under way.

E. E. Austin, H. F. Castro-Gonzalez, K. E. Sides, C. W. Schadt, and A. T. Classen. "Assessment of 10 years of CO_2 fumigation on soil microbial communities and function in a sweetgum plantation," **Soil Biology & Biochemistry** 41: 514–520 (2009), DOI: 10.1016/j.soilbio.2008.12.010.

Differential characterization of carbon sources for aboveground and belowground plant tissues

The role of dissolved organic carbons (DOCs) in the buildup of soil organic carbon pools is still not well known, but DOCs are thought to play a role in the transport of carbon to a greater depth where it becomes more stable. Using mesocosms with constructed soil profiles that simulate realistic conditions but allow for manipulation of environmental factors, ORNL scientists enriched

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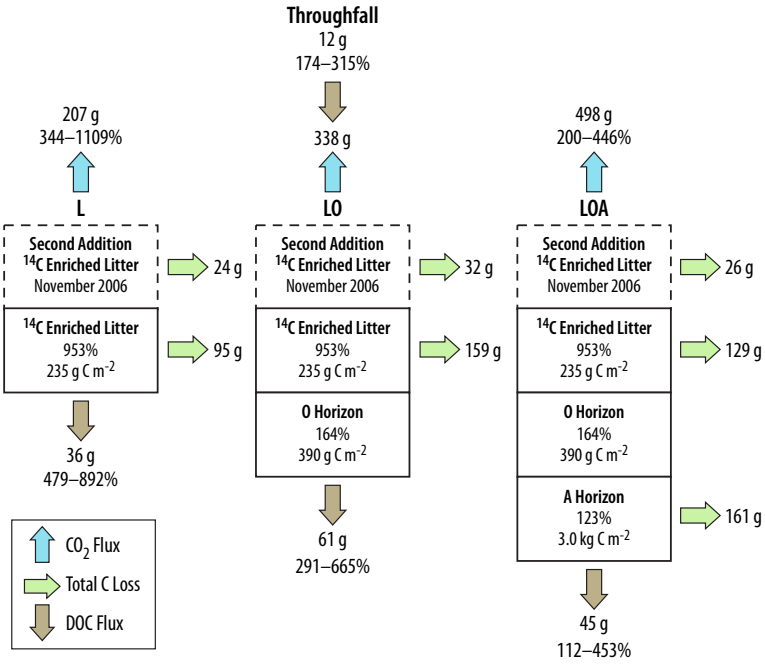
leaf litter with radioactive carbon-14 (^{14}C) and identified mechanisms of DOC movement and retention within the humus (stable organic matter) and surface mineral layers of forest soils. The mesocosms were placed in the field for 17 months, during which time fluxes and ^{14}C content of DOC and CO_2 were measured, as well as changes in ^{14}C concentration in leaf litter and bulk soil carbon pools. The results showed that substantial leaching of newly formed DOC from fresh litterfall was not absorbed by the soil humus layer but instead was efficiently transferred to the mineral soil. DOC transport to and retention by surface soils was extensive, yet net annual DOC input was small compared with carbon stocks and, therefore, not important for changes in soil carbon on an annual timescale.



Characterizing the use of carbon reserves in trees is important for understanding local, regional, and global carbon cycles. In another study using ^{14}C release, ORNL scientists estimated that the mean age of stored carbon used to grow both leaf buds and new roots in a temperate deciduous oak forest is 0.7 years and that about 55% of new-root growth annually comes from stored carbon. The calculated mean age of carbon used to grow new-root tissue is 0.4 years. New roots contain a lot of stored carbon, but they are young in age. In addition, the researchers found that the type of structure used to model stored carbon input is important. Model structures that did not include storage, or that assumed stored and new carbon mixed well (within root or shoot tissues) before being used for root growth, did not fit the data nearly as well as the use of a distinct carbon storage pool. The mean age of carbon in new-root tissues in three additional forest sites in North America and Europe was less than 1–2 years. Models of tissue carbon dynamics must take stored reserves into account, particularly for pulse-labeling studies and root turnover in less than a year.

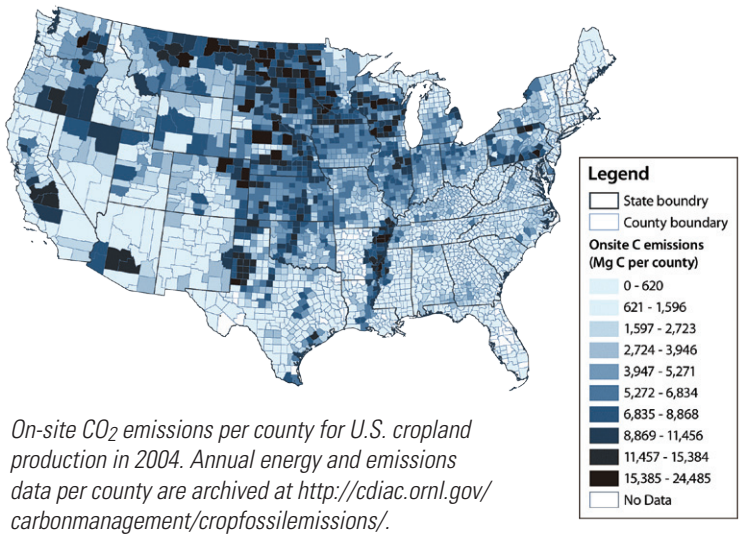
M. Fröberg, P. J. Hanson, S. E.Trumbore, C. W. Swanston, and D. E. Todd. "Flux of carbon from ^{14}C-enriched leaf litter throughout a forest soil mesocosm," **Geoderma** 149:181–188 (2009).

J. B. Gaudinski, M. S. Torn, W. J. Riley, C. Swanston, S. E. Trumbore, J. D. Joslin, H. Majdi, T. E. Dawson, and P. J. Hanson. "Use of stored carbon reserves in growth of temperate tree roots and leaf buds: analyses using radiocarbon measurements and modeling," **Global Change Biology** 15: 992–1014 (2009).

Research Highlights

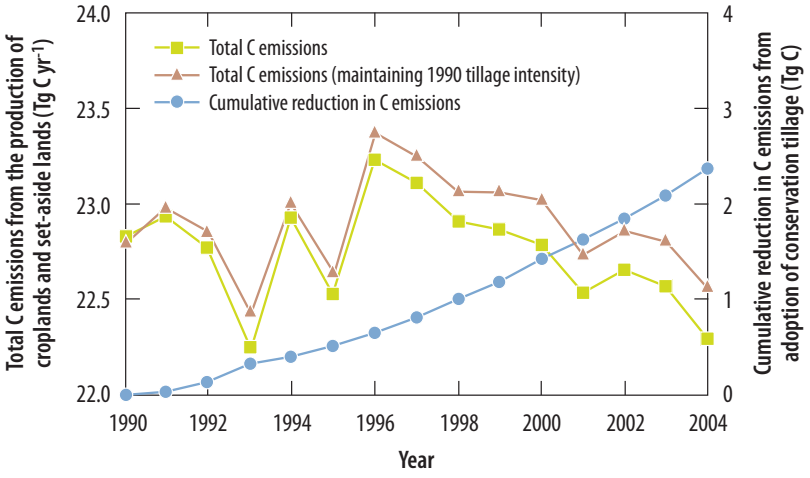
Trends in energy consumption and CO_2 emissions from cropland production

Changes in cropland production and field management influence energy consumption and emissions of CO_2 from fossil-fuel combustion. The objective of this study was to investigate changes in energy use and fossil-fuel CO_2 emissions associated with cropland management from 1990 to 2004. Cropland management scenarios include over 3500 unique combinations of planted crop species, production inputs, and tillage operations. Changes in cropland management are impacted by changes in policy (e.g., farm bills and energy bills), weather, and technology. These changes cause significant shifts in energy use and CO_2 emissions from U.S. croplands.



On-site CO_2 emissions per county for U.S. cropland production in 2004. Annual energy and emissions data per county are archived at http://cdiac.ornl.gov/carbonmanagement/cropfossilemissions/.

A method was developed to calculate on-site and off-site energy and CO_2 emissions for crop practices at the county scale. Energy consumption and emissions occur on-site from the operation of farm machinery and off-site from the manufacture and transport of cropland production inputs, such as fertilizers, pesticides, and agricultural lime. Estimates of fossil-fuel consumption and associated CO_2 emissions for crop practices enable (1) the monitoring of energy and emissions with changes in land management and (2) the calculation and balancing of regional and national carbon budgets.



Total fossil-fuel CO_2 emissions from U.S. cropland production compared to total emissions estimated while holding conservation tillage adoption steady after 1990, and cumulative difference between the two scenarios. Conservation tillage includes reduced tillage and no-till operations.

ORNL scientists estimated on-site and off-site energy use and CO_2 emissions resulting from cropland production. Depending on the crop being planted and the suite of production inputs, croplands using reduced tillage practices generally consumed less energy and produce less CO_2. Abrupt changes in emissions were also found to be affected by extreme weather events, as well as

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agricultural policies and commodity prices. While these trends were already widely known, the development and analysis of these data enable the monitoring of changes in energy and CO_2 emissions associated with cropland management and with carbon sequestration strategies (e.g., reduced tillage) per year and per county.

Results indicate on-site energy use and total energy use (i.e., the sum of on-site and off-site) on U.S. croplands in 2004 ranged from 1.6–7.9 GJ ha^{-1} yr^{-1} and from 5.5–20.5 GJ ha^{-1} yr^{-1}, respectively. On-site and total CO_2 emissions in 2004 ranged from 23–176 kg C ha^{-1} yr^{-1} and from 91–365 kg C ha^{-1} yr^{-1}, respectively. During the period of this analysis (1990–2004), national total energy consumption for crop production ranged from 1204–1297 PJ yr^{-1} (petajoule = 1×10^{15} joule) with associated total fossil CO_2 emissions ranging from 22.0–23.2 Tg C yr^{-1} (teragram = 1×10^{12} gram). The annual proportion of on-site CO_2 to total CO_2 emissions changed depending on the diversity of crops planted. Adoption of reduced tillage practices in the United States from 1990 to 2004 resulted in a cumulative net emissions reduction of 2.4 Tg C.

R. G. Nelson, C. M. Hellwinckel, C. C. Brandt, T. O. West, D. G. De La Torre Ugarte, and G. Marland. "Energy Use and Carbon Dioxide Emissions from Cropland Production in the United States, 1990–2004," **Journal of Environmental Quality** 38: 418–425 (2009).

New methods for analyzing photosynthetic CO_2 response in C_3 leaves

C_3 plants, which account for more than 95% of the earth's plant species, take in CO_2 through their open stomata and, using the energy of sunlight and water, synthesize plant tissue for growth. In the first stage of photosynthesis to make carbohydrates, C_3 plants produce the three-carbon compound phosphoglyceric acid, the first stable product of the plants' carbon fixation and the basis for the plants' name. Researchers have been modeling the photosynthetic responses of C_3 plants to rising atmospheric CO_2 concentrations to predict the impacts on leaf physiology and behavior. However, certain basic quantities called parameters must be provided in order to run the models properly. These parameters are determined from measurements of photosynthetic CO_2 response (A/Ci) curves through a numerical optimization process.

ORNL scientists have developed new analytical methods to better determine the photosynthetic parameters for C_3 leaves and the production of carbon-cycle model inputs. Extant A/Ci curve fitting approaches, including a recently proposed simultaneous estimation method, were shown to have crucial shortcomings that prevent them from reliably estimating parameters in the Farquhar-von Caemmerer-Berry (FvCB) model. The shortcomings include a necessary fixing of the ratio of two key parameters without input from data, non-optimal fitting, and inconsistency with the FvCB formulation (points of one limitation state may turn out to be those of another limitation state after the parameters are estimated). These shortcomings are responsible for the failure of extant approaches to recognize the unusual structural characteristics of the FvCB model that invalidate the use of conventional optimization algorithms.

A detailed model structural analysis was conducted from a parameter estimation point of view. The ORNL scientists identified where and how FvCB optimization might fail and established

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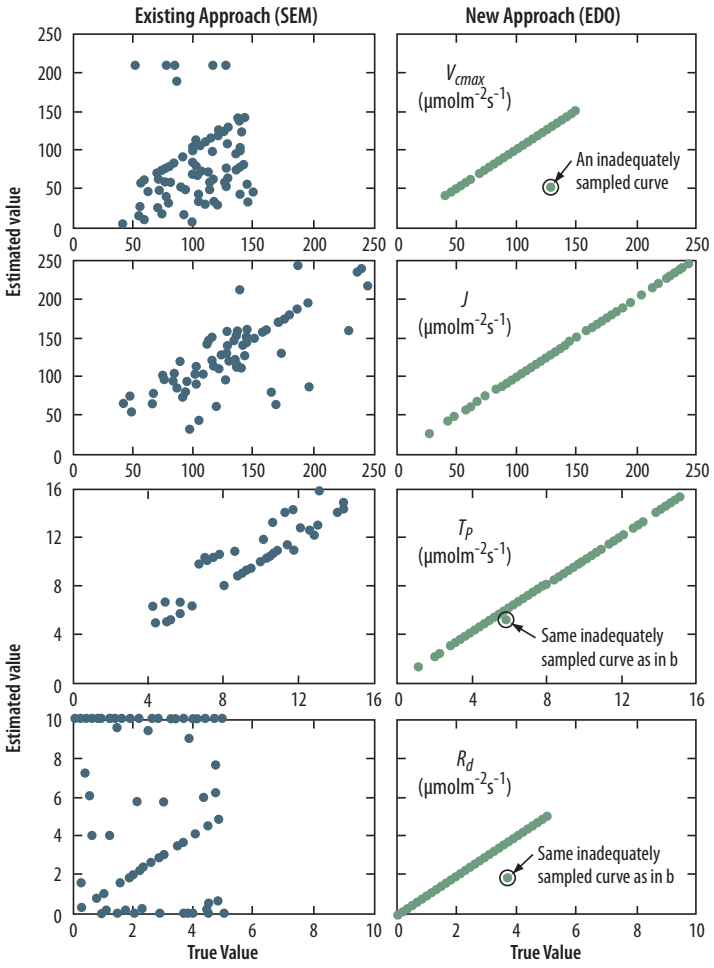
which parameters or parameter expressions can be uniquely resolved and which cannot under different scenarios of limitation states. The insight gained through this effort led ORNL scientists to develop the Exhaustive Dual Optimization (EDO) approach, which takes into consideration the uniqueness of the FvCB structure. EDO consists of limitation state combination optimization (LSCO) and parameter optimization (PO) with PO nested within LSCO. EDO combines numerical techniques with established knowledge of photosynthetic CO_2 response in a manner consistent with the FvCB structure.

Additionally, the model structural analysis pointed to procedures for informative A/Ci curve measurements. The curvature (nonlinear) region of an A/Ci curve was found to be crucial. Prior knowledge of a species or exploratory measurements should be used first to establish the broad pattern of an A/Ci curve and to estimate the likely location of the curvature. Relatively dense measurements should then be made preferentially within the curvature region.

Model simulations, sampled A/Ci curves, and chlorophyll fluorescence measurements of different tree species were used to demonstrate the reliability and advantage of EDO. An interactive website has been set up for users interested in applying this new technique (http://leafweb.ornl.gov).



The progress of ORNL scientists has received high remarks from editors and reviewers of *Plant, Cell and Environment*, a leading international scientific journal. An excerpt follows:

"The methods (developed by ORNL scientists) . . . may constitute a very significant advance in the estimation of the parameters of the FvCB model of carbon assimilation, and could be the definitive solution to a longstanding problem. They might be of even broader importance, in the study of change-point models in general . . . very real possibility that the authors have achieved a remarkable breakthrough."

L. Gu, S. G. Pallardy, K. Tu, B. E. Law, and S. D. Wullschleger. "Reliable estimation of biochemical parameters from C_3 leaf photosynthesis-intercellular carbon dioxide response curves," **Plant, Cell and Environment** (accepted).

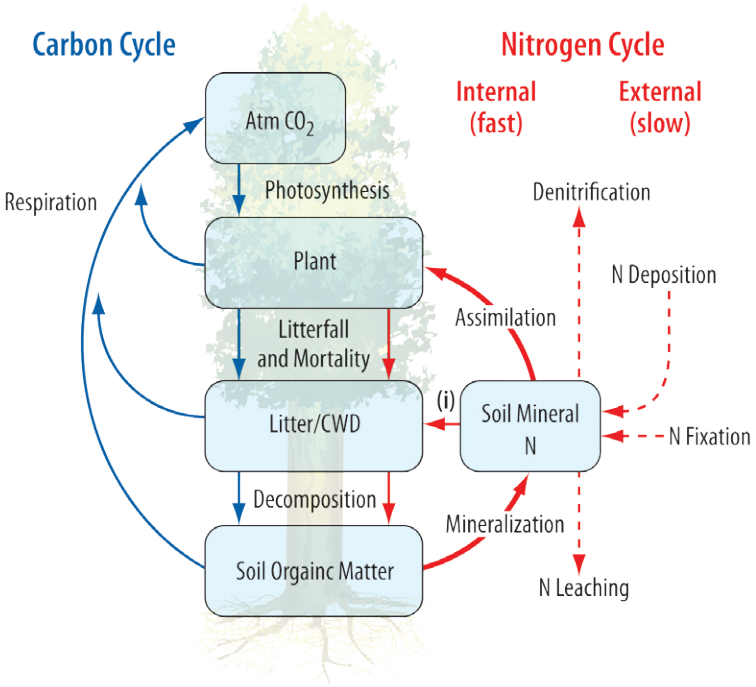
Research Highlights

Refining model forecasts of climate change and global warming

The uptake of CO_2 by plants and land ecosystems depends on the availability of nutrients such as nitrogen to support new growth. Recent studies conducted by Peter Thornton of the Environmental Sciences Division and a team of climate scientists suggest that the relationship between global climate change and the carbon cycle is fundamentally influenced by the carbon–nitrogen cycle interactions.

By incorporating carbon–nitrogen interactions in a global climate model, Thornton and his team have demonstrated the significant role that the carbon–nitrogen cycle plays in CO_2 uptake by plants and on land. Based on their research, they have determined that stimulation of plant growth due to rising CO_2 over the next century may be two to three times less than previously predicted due to a lack of available nutrients, such as nitrogen. Less CO_2 being absorbed by vegetation would result in more CO_2 in the atmosphere.

This reduction in the CO_2 fertilization effect is partly offset by another carbon–nitrogen cycle interaction. Warming under radiatively forced climate change leads to fertilization of plant growth by mineralization of nitrogen, which is directly associated with the decomposition of soil organic matter. Although there is evidence that nitrogen availability may increase as a result of warming-induced decomposition, it will not be enough to offset the reduction in CO_2 fertilization of plant growth. Levels of atmospheric CO_2 could be even higher than predicted by this model, since consideration has not yet been given to changing land use patterns and shifts in types of vegetation.



Schematic illustrating feedback pathways coupling terrestrial carbon and nitrogen cycles with the Community Land Model (CLM-CN). Blue arrows show, in general, the processes represented in previous carbon-only land model components: plant carbon uptake by photosynthesis draws down atmospheric CO_2; litterfall and plant mortality pass biomass from plant to litter and coarse woody debris (CWD); decomposition of fresh litter generates soil organic matter; respiration by both plants and heterotropic organisms returns CO_2 to the atmosphere. Orange arrows show the additional processes represented in the coupled carbon-nitrogen land model, differentiated here between rapid internal cycling (solid arrows) and slower fluxes between land pools, the atmosphere, and groundwater (dashed arrows). The critical feedback pathway connecting heterotrophic respiration with plant growth is highlighted as a thick red arrow: decomposition of soil organic matter not only releases CO_2 to the atmosphere, it also releases nitrogen from the organic matter (mineralization) in forms that can then be taken up by plants (assimilation). Plant nitrogen uptake competes with the demand for mineral nitrogen from heterotrophic organisms decomposing fresh litter. In this figure, immobilization is abbreviated (i).

Research Highlights

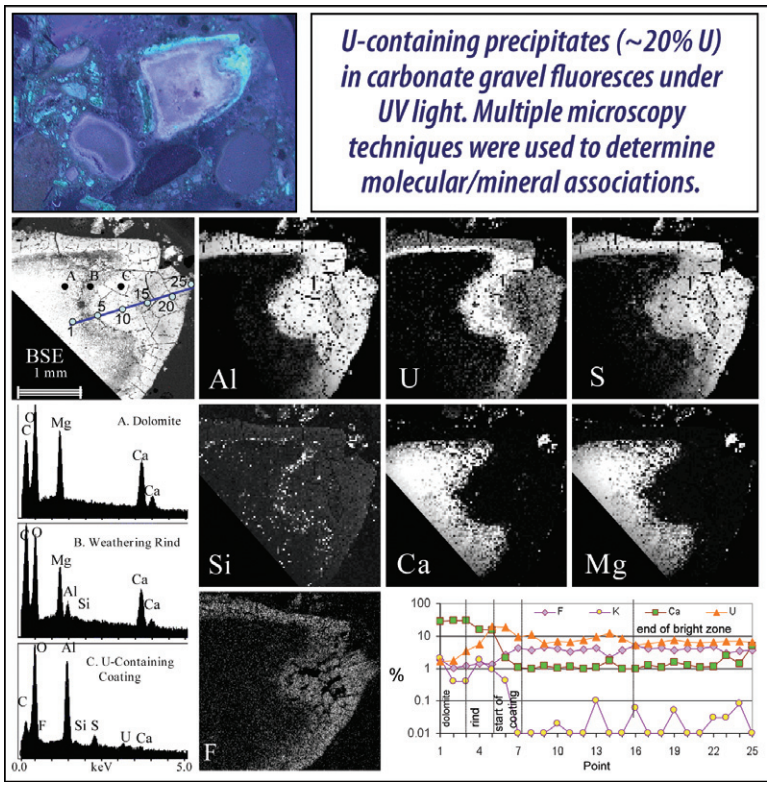
Including some kind of nutrient dynamics in global climate models will lead to more accurate climate change predictions, according to Thornton, who also notes that "in order to do these experiments in the climate system model, expertise is needed in the nitrogen cycle, but there is also a need for climate modeling expertise, the ocean has to be involved properly, the atmospheric chemistry . . . and then there are a lot of observations that have been used to parameterize the model." The ability to handle the complexities of climate models has been facilitated by the ORNL Leadership Computing Facility.

This breakthrough in reducing the uncertainty associated with atmospheric CO_2 and climate change modeling is one more step toward achieving a more accurate and realistic prediction of the future of the earth's climate.

P. E. Thornton, S. C. Doney, K. Lindsay, J. K. Moore, N. Mahowald, J. T. Randerson, I. Fung, J.-F. Lamarque, J. J. Feddema, and Y.-H. Lee. "Carbon–nitrogen interactions regulate climate-carbon cycle feedbacks: results from an atmosphere-ocean general circulation model," **Biogeosciences** 6: 2099–2120 (2009).

SUBSURFACE SCIENCE

Laboratory collaboration elucidates uranium characterization within carbonate gravel



Through the collaborative efforts of scientists at Oak Ridge National Laboratory and Argonne National Laboratory, important molecular, mineralogical, and field lithologic associations of uranium-containing precipitates in carbonate gravel fill from a former DOE waste disposal site were analyzed. The study was conducted to assess the effectiveness of remedial actions used to remove uranium from the subsurface.

Using X-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), the scientists determined that the uranium coating the gravel is hexavalent and that the uranyl is coordinated by carbonate, the structure of which resembles a split K^+-like shell, similar to

Research Highlights

grimselite. In other areas the structure was found to more closely resemble a single Ca^{2+}-like shell, like liebigite or andersonite.

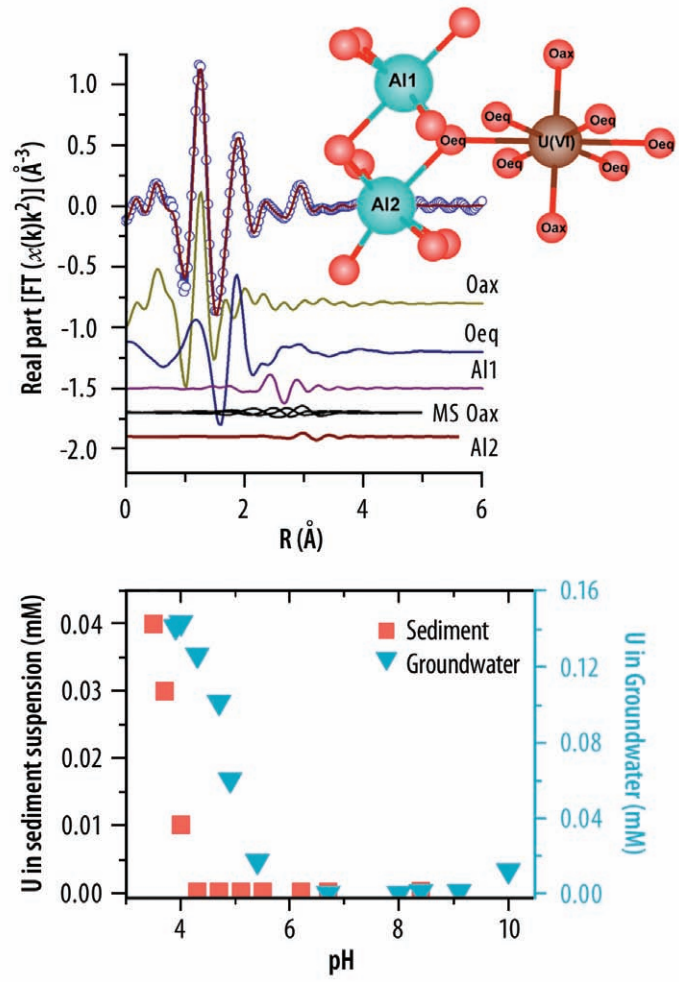
The results of this study suggest the effectiveness of high pH carbonate gravel as a potential treatment media in the removal and sequestration of uranium from groundwater. Carbonate minerals were found to effectively remove uranium from acidic contaminated groundwater containing high levels of Al^{3+}, Ca^{2+}, NO_3^-, and SO_4^{2-} by raising the groundwater pH, which induced precipitation of uranium.

D. H. Phillips, D. B. Watson, S. D. Kelly, B. Ravel, and K. M. Kemner. "Deposition of Uranium Precipitates in Dolomitic Gravel Fill," **Environmental Science & Technology** 42(19): 7104–7110 (2008).

A new way to fix uranium and technetium pollutants in a contaminated acidic environment

Uranium and technetium are among the most prevalent radionuclide contaminants found in soils and groundwater across the U.S. Department of Energy complex. Despite many years of research and development, a cost-effective remedial approach to removing these pollutants is still lacking, particularly under strong acidic pH conditions where many technologies such as bioremediation do not work well.

Scientists from Oak Ridge National Laboratory, Argonne National Laboratory, and the University of Oklahoma found a simple yet effective technique for fixing these radioactive pollutants in a highly contaminated acidic soil located at the Y-12 National Security Complex in Oak Ridge, Tennessee. The technique takes advantage of the acidic groundwater that contains high levels of metal ions such as aluminum, nickel, and cobalt (also toxic metals). The ions were slowly converted to hydroxide solid precipitates by controlled neutralization using a strong base such as sodium hydroxide. The scientists found that >94% of soluble uranium (as UO_2^{2+}), >83% of technetium (as TcO_4^-), and >90% of nickel (as Ni^{2+}) and cobalt (Co^{2+}) were readily precipitated out together with aluminum when the pH was raised to above 4.5. Because the precipitated uranium and technetium form strong chemical bonds with hydroxide solids,



Research Highlights

both were found to be stable against leaching as long as an adequate pH condition was maintained (e.g., from 4.5 to 7.5). However, extremely low or high pH (with carbonate) conditions could break down the precipitated solid forms into their toxic ionic forms that are soluble in groundwater.

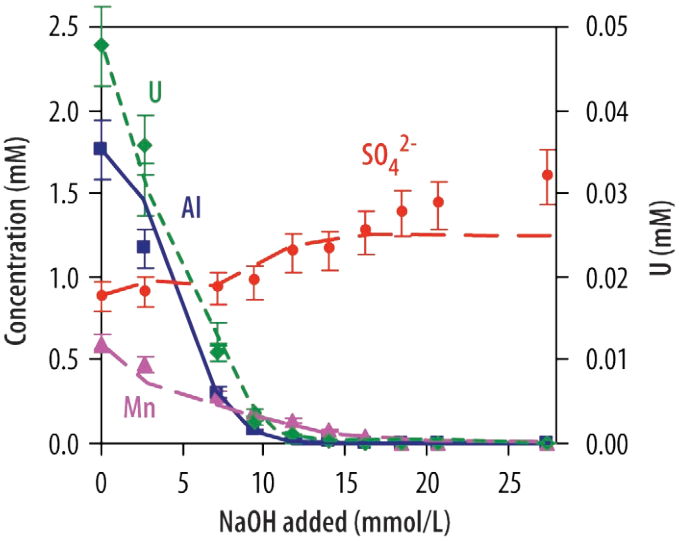
The results of this study show that as long as a pH of >4.5 and a low carbonate level are maintained, both uranium and technetium can be effectively sequestered in solids. It is thus feasible and effective with controlled pH manipulation to remediate uranium- and technetium-contaminated soils and groundwater and prevent uranium and technetium from migrating to the surrounding environment.

W. Luo, S. D. Kelly, K. M. Kemner, D. Watson, J. Zhou, P. M. Jardine, and B. Gu. "Sequestering uranium and technetium through co-precipitation with aluminum in a contaminated acidic environment," **Environmental Science & Technology** 43: 7516–7522 (2009).

New modeling approach to assess the effect of pH on removal of trace metals and radionuclides during remedial actions at DOE sites

Wastes containing strong acid, inorganic, organic, and radioactive materials released during nuclear material production and processing are the source of extensive subsurface contamination at U.S. Department of Energy facilities. Disposal of such wastes in the past has resulted in contaminated groundwater with a low pH and high concentrations of aluminum, iron, calcium, magnesium, manganese, and nitrate; various trace metals such as nickel and cobalt; and radionuclides such as uranium and technetium. Aquifer pH has been found to have a strong effect on many geochemical reactions that control contaminant mobility; therefore, understanding the acid–base behavior of a soil–solution system is critical to predicting metal transport under variable pH conditions.

To provide an effective means of simulating the effects of pH on inorganic subsurface contaminants, scientists from ORNL and the University of Tennessee investigated the modeling of the geochemical reactions (including various aqueous phase, precipitation/dissolution, and adsorption/desorption reactions) during base addition to acidic contaminated sediments. Such modeling can be used to predict how pH affects aqueous- and solid-phase concentrations of metals and anions in an effort to develop strategies for the remediation of contaminated sites at DOE facilities.



Concentrations of metals and anions during titration

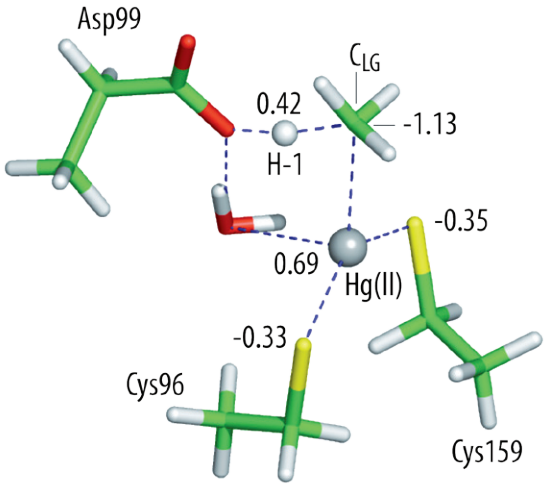
Research Highlights

Batch titration experiments of contaminated sediments were performed by the scientists to evaluate the geochemical reaction dynamics under varying pH conditions. To simulate the soil buffer and pH-dependent cation/anion exchange capacities, the aquifer solids were treated as polyprotic acid/base controlled by mineral precipitation/dissolution reactions. The pH and aqueous- and solid-phase concentrations of metals (e.g., aluminum, calcium, magnesium, strontium, manganese, nickel, cobalt, uranium) and anions (e.g., uranium and sulfate) simulated during base additions closely matched experimental data. The results of this study therefore suggest that this geochemical model could potentially be used to predict the acid-base behavior of the sediment-solution system under variable pH conditions.

F. Zhang, W. Luo, J. Parker, J. C. Parker, B. P. Spalding, S. C. Brooks, D. B. Watson, P. M. Jardine, and B. Gu. "Geochemical modeling of reactions and partitioning of trace metals and radionuclides during titration of contaminated acidic sediments," **Environmental Science & Technology** 42: 8007–8013 (2008).

Greater understanding of bacterial enzymes may lead to better mercury bioremediation

Mercury is a significant environmental contaminant that is toxic to both plant and animal species. While there are natural avenues for mercury deposition in the environment (e.g., volcanic eruptions, geothermal phenomena, and weathering of minerals), many industrial processes such as burning of fossil fuels also contribute to the environmental accumulation of mercury. Once in the environment, mercury is converted to organomercurials, or molecules containing mercury-carbon bonds, such as methylmercury, which are much more toxic and, worse, bioaccumulate in various plants and animals where they are concentrated as they move up the food chain.



Transition state structure for the energetically preferred mechanism of MerB. Selected atomic charges are shown.

Because of this bioaccumulation process, even though many countries have been controlling their mercury emissions for some time, mercury continues to accumulate in various animal populations. And due to industrialization in underdeveloped countries, fossil fuel emissions of mercury are expected to increase in the next 20 to 30 years. Thus, finding solutions to mercury contamination is becoming more critical.

It has been known for some time that some bacteria are not only resistant to mercury poisoning but in fact can convert the highly toxic organomercurials to more benign forms of mercury through a catalytic demethylation process. The bacterial enzyme, organomercurial lyase, MerB, is capable of detoxifying a wide range of organomercurials, including the highly toxic methymercury, by breaking the Hg-C bond. However, many of the details of the process are not well understood.

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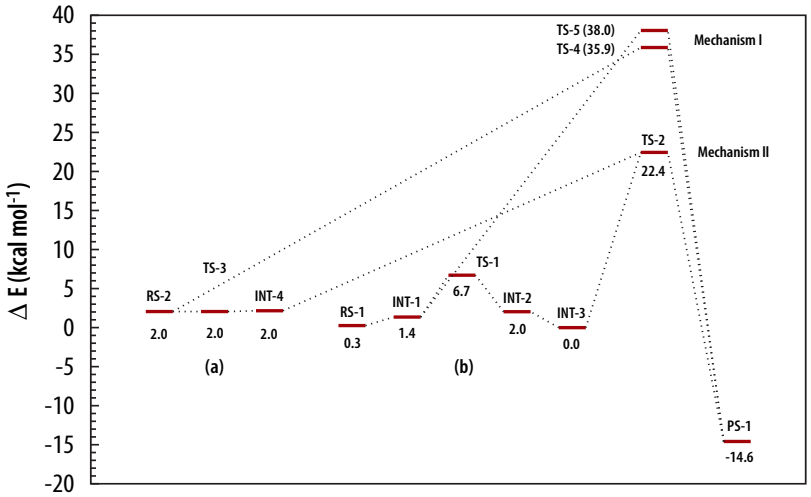
Recently a team of scientists from ORNL, the University of Tennessee, the University of Georgia, and the University of California at San Francisco used structural models of the MerB enzyme developed from new X-ray crystallographic data to narrow the investigation to the two most likely reaction mechanisms and then used quantum chemical calculations to confirm their theories.

The authors calculated the energy required to break the mercury-carbon bond in methylmercury by two different mechanisms. One of the calculated mechanisms agreed well with experimentally measured energies, providing evidence that the mechanism was likely to be correct. Further tests of the mechanism were performed, in which activation energies were computed for two other organomercurials. Again the results were found to agree well with experiments.



Total energy profiles for the two mechanisms investigated calculated using density functional theory methods

Mercury is known to bind strongly to sulfur, and MerB works by luring methylmercury into its active site with sulfur-containing cysteine amino acids. Two cysteines must coordinate, or bond, with methylmercury to weaken the mercury-carbon bond. Meanwhile, a third amino acid, aspartic acid, delivers a proton that breaks the bond.

These findings contribute to the fundamental understanding of the biological systems and processes involved in the transformation of mercury species in the environment. Such information may be useful in the future design of synthetic catalysts for detoxifying mercury-polluted streams and rivers.

J. M. Parks, H. Guo, C. Momany, L. Liang, S. M. Miller, A. O. Summers, and J. C. Smith. "Mechanism of mercury-carbon protonolysis in the organomercurial lyase MerB," **Journal of the American Chemical Society** 131(37): 13278–13285 (September 2009).

Natural humic substances affect the dissolution and mobilization of reduced uranium under anaerobic conditions

The stability and mobility of uranium are strongly influenced by its oxidation state: hexavalent uranium [U(VI)] is soluble and hence mobile in soils and water, while tetravalent uranium [U(IV)] is relatively insoluble and immobile. In the last decade scientists have discovered a number of bacteria capable of reducing U(VI) to U(IV), decreasing its solubility and sequestering it in place, a potentially cost-effective remediation solution for contaminated sites. However, because the reduced uranium is not contained in any physical barriers and is left in place, concerns remain related to its long-term stability and the possibility of reoxidation and remobilization under varying environmental conditions during the long stewardship required for contaminated sites.

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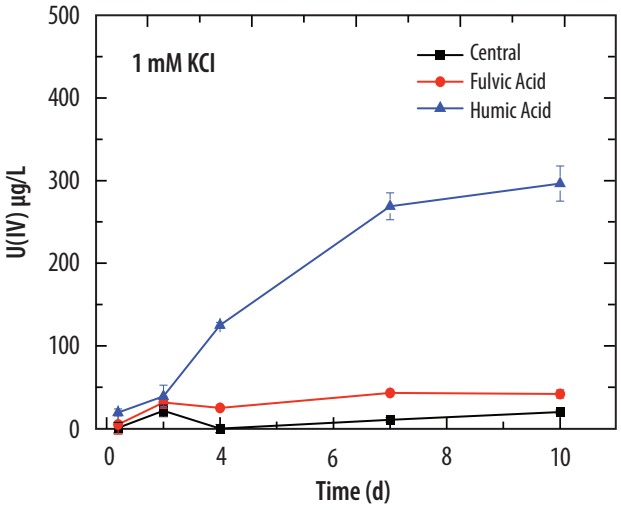
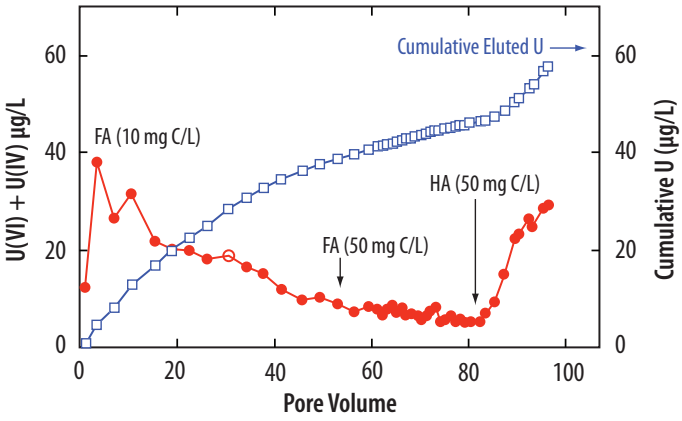
Previous studies have in fact documented reoxidation and remobilization of uranium in the presence of dissolved oxygen, leading to the belief that maintaining a strict anaerobic environment is needed to prevent reoxidation of U(IV). However, in other studies humic substances—specifically the naturally forming ligands in soil and groundwater—have been found to enhance the dissolution and/or mobilization of U(IV) by forming soluble complexes, even under strict anaerobic conditions. Natural humics therefore would seem to present a challenge to maintaining the long-term stability of uranium in the environment.



Increased dissolution of bioreduced U(IV) by humics

To further explore and document the viability of in situ bioreduction for sequestration of environmental uranium, scientists at ORNL initiated a study to investigate the effects of natural humic substances on the dissolution and mobilization of U(IV) and U(VI) in a contaminated sediment. The sediment was biologically reduced to simulate field remedial conditions before batch kinetic and column flow-through experiments were performed.

The results confirmed the ability of humic substances to dissolve U(IV) by complexation under reducing conditions, although the dissolution process appears to be slow even in the presence of relatively high levels of humics. The study concludes that the dissolution and mobilization of reduced U(IV) can be a long-term concern, especially in the presence of strong complexing agents such as humic acid. Seasonal variations in hydrogeologic conditions and land-management practices, yet to be explored, may also contribute to the viability or mobility of U(IV) in the environment.

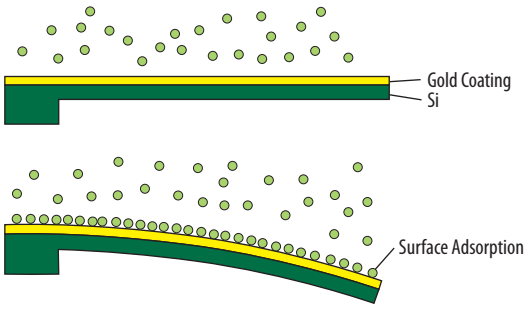


Elution profile and cumulative amount of uranium leached from a bioreduced sediment column by varying concentrations of humics (humic acid and fulvic acid)

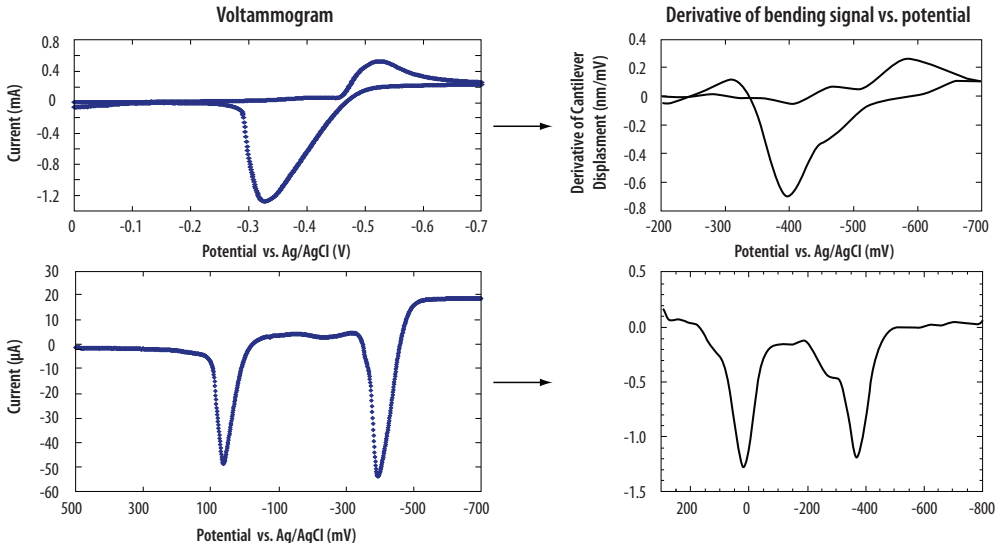
W. Luo and B. Gu. "Dissolution and mobilization of uranium in a reduced sediment by natural humic substances under anaerobic conditions," **Environmental Science & Technology** 43: 152–156 (2009).

Research Highlights

Selective detection of metal ions using a microcantilever electrode



Microcantilevers can be highly sensitive chemical sensors if a chemical process that changes surface free energy is confined to one side of the cantilever beam. Microfabricated silicon microcantilevers coated with gold on one side have been used as working electrodes in a three-electrode electrochemical arrangement. In addition to electrochemical current, cantilever bending has been used as a signal for monitoring electrode reactions on the cantilever. The microcantilever bending was measured by an optical beam deflection method as the surface potential scanned and electrochemical reactions occurred on the surface.



This research shows that an electrochemical reaction on the microcantilever surface can be used as a sensitive technique for specific ions based on the electrochemical potential of the redox species. Scientists at ORNL have demonstrated this technique for the detection of lead and copper ions in a solution using cyclic voltammetry and liner sweep stripping voltammetry. This process is extremely sensitive to initial monolayers of adsorbate and is not controlled by the diffusion process. While this research focuses on lead and copper, the technique is suitable for a wide range of redox-active analytes including mercury, cadmium, and nickel.

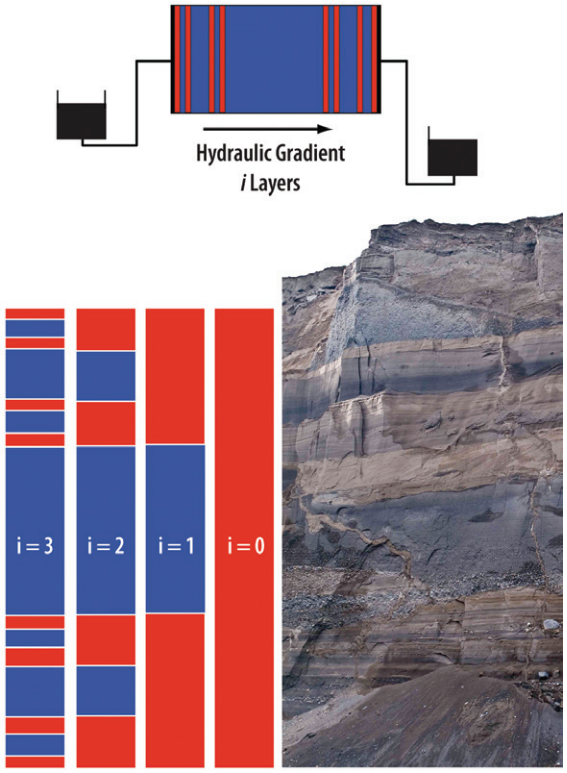
A. F. Bange, G. M. Brown, L. R. Senesac, and T. G. Thundat. "Voltammetry of the Pb/Pb^{2+} Redox Couple Using Gold Microcantilever Electrodes," **ECS Trans.** 16(11): 147 (2008).

A. F. Bange, G. M. Brown, L. R. Senesac, and T. G. Thundat. "Stripping Voltammetry pf Pb and Cu Using a Microcantilever," **Surface Science** 603: L125–L127 (2009).

Research Highlights

Cantor bar composite medium model used to predict hydraulic properties of unsaturated layered sediments

Scale dependence of basic hydraulic parameters is a major obstacle for the prediction of water flow and contaminant transport at many contaminated U.S. Department of Energy sites because parameters obtained at the laboratory column scale may not be applicable to the field scale. While observing a cliff of rocks or sediments from a distance, for example, a number of sedimentary layers might be recognized. Getting closer, each individual layer can be further subdivided into a number of smaller layers, and so on. The relationship between the whole package of sediment layers and the individual layers, however, is constant regardless of the spatial scale. Fractals are geometric models comprised of irregular or fragmented elements that repeat themselves across a wide range of spatial scales (i = n). Since fractal parameters are scale invariant, they are a natural choice for inclusion in physically based models designed to predict properties or processes at one scale based on information collected at another scale.



Scientists at ORNL used a physically based Cantor bar model to predict the effective hydraulic parameters of unsaturated layered sediments at a range of spatial scales using a composite medium approach. Numerical simulation results showed that this approach works well for steady-state unsaturated flow through a layered sequence comprised of thin layers of fine sand (blue) interbedded within a coarse sand (red). As the hydraulic gradient through multiple layers (i = n) increased, the effective parameters deviated from predictions using the composite medium model. Individually layered and composite parameters, however, were similar. Together with a composite medium approach, the Cantor bar model can be used to predict effective hydraulic properties as a function of spatial scale. Further work is necessary to validate the model predictions by performing measurements at different scales, and to assess the applicability of this approach to transient flow conditions.

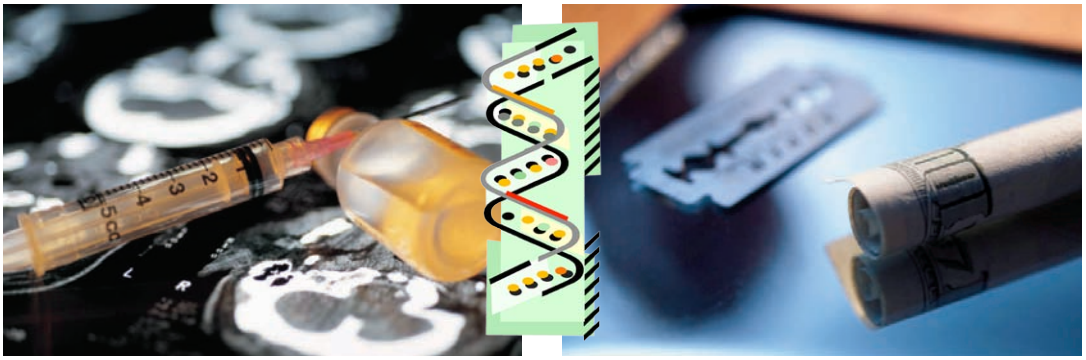
G. Tang, E. Perfect, E. H. Vanden Berg, M. A. Mayes, and J. C. Parker. "Estimating Effective Hydraulic Parameters of Unsaturated Layered Sediments Using a Cantor Bar Composite Medium Model," **Vadose Zone Journal** 7(2): 493–499 (2008); www.vadosezonejournal.org.

Research Highlights

BIOLOGICAL SYSTEMS

Enhancing SNP arrays for genes relevant to addiction

A high-throughput systems genetic analysis revealed many new genes associated with addiction-related behaviors. In collaboration with investigators funded by the National Institute on Drug Abuse, ORNL scientists identified these genes and prioritized them for addition to human single nucelotide polymorphism (SNP) genotyping arrays tailored to address disorders of addiction.



Addiction is thought to be influenced by complex interactions among many relevant genes and pathways. The team led by Washington University in St. Louis assembled a list of 486 biologically relevant genes nominated by a panel of experts on addiction, and the ORNL team added 424 genes that showed evidence of being associated with addiction through quantitative trait loci mapping and gene co-expression analysis in mice. The results showed that all the commercial SNP platforms considered must be supplemented to cover comprehensively the genes that are biologically relevant to addiction in African, Chinese, European-American, and Japanese populations.

A publicly available SNP database was developed that is annotated using numeric scores to indicate the extent to which individual SNPs are biologically relevant to addiction. The prioritization scores incorporate factors such as SNP/gene functional properties, data from mouse systems genetics, and measures of human/mouse evolutionary conservation. HapMap genotyping data were used to determine if an SNP is tagged by a commercial microarray through linkage disequilibrium (LD). The combination of biological prioritization scores and LD tagging annotation will enable addiction researchers to supplement commercial SNP microarrays to ensure comprehensive coverage of biologically relevant regions.

This effort illustrates ORNL's ability to integrate convergent genetic and genomic data and prioritize functionally relevant genes. The approaches used will help other investigators supplement these arrays, target specific genomic regions such as genes and linkage regions, and improve the general selection of SNPs for genetic studies of addiction based on the criterion of "biological role in addiction."

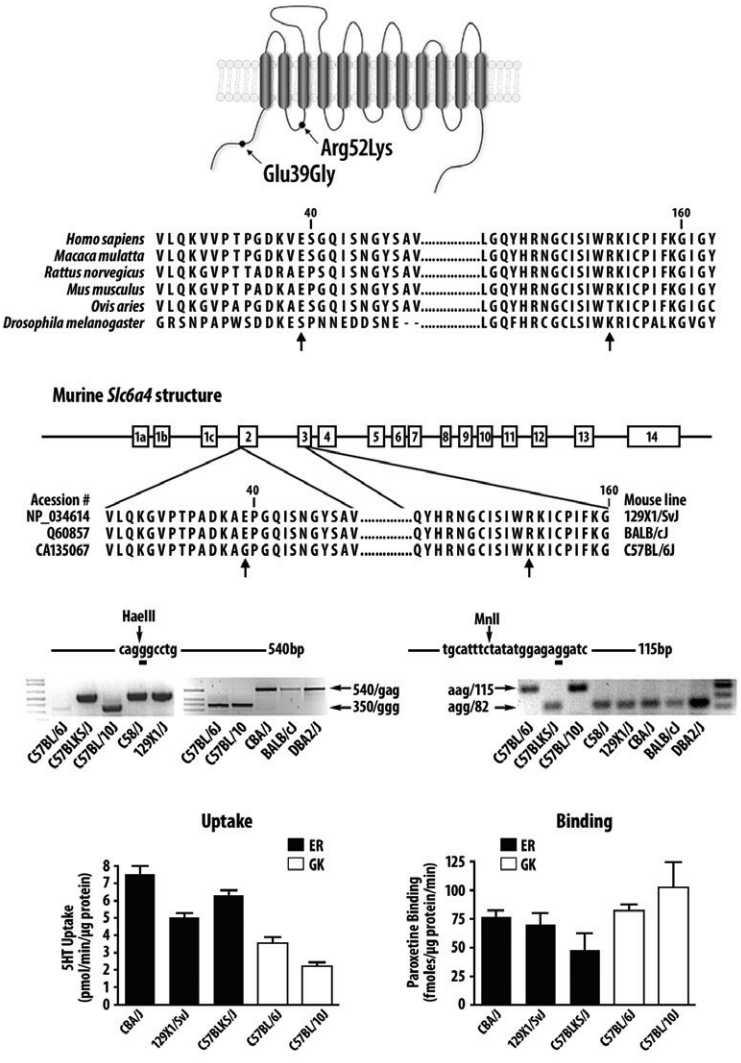
S. F. Saccone, L. J. Bierut, E. J. Chesler, P. W. Kalivas, C. Lerman, N. L. Saccone, G. R. Uhl, C-Y. Li, V. M. Philip, H. J. Edenberg, S. T. Sherry, M. Feolo, R. K. Moyzis, and J. L. Rutter. "Supplementing high-density SNP microarrays for additional coverage of disease-related genes: Addiction as a paradigm," **PLoS ONE** 4(4): e5225 (2009).

Research Highlights

Altered SERT functioning in RI mouse populations

The chemical serotonin is transported to neurons in the nervous system by the protein human serotonin transporter (hSERT, *SLC6A4*), which figures prominently in the origin and treatment of many common neurobehavioral disorders including anxiety, alcoholism, depression, autism, and obsessive-compulsive disorder.

Elissa Chesler of the Biosciences Division was part of a team that used naturally occurring genetic polymorphisms in recombinant inbred (RI) lines of mice to identify sets of genes associated with altered SERT function. The work used reference mouse populations and systems genetics to discover the effects of segregating genetic polymorphisms based on predictions from computation.



The researchers found that some mouse strains contain a variant form of SERT known as "GK," which has a reduced ability to transport serotonin. Most mouse strains contain a SERT variant known as "ER," which is identical to hSERT. Using RI mice, the team found that GK mice performed differently from ER mice on tests related to depression and anxiety. Using an "in silico" (computational) approach, the researchers analyzed a public database of traits originally compiled by Dr. Chesler and associated with the GK variant in mouse populations. They identified several traits affected by the GK SERT variation, including those associated with alcohol consumption and dopamine use. They also found that mice with the GK variant had significantly higher levels of iron in their brains, indicating a possible link between brain iron levels and SERT functioning.

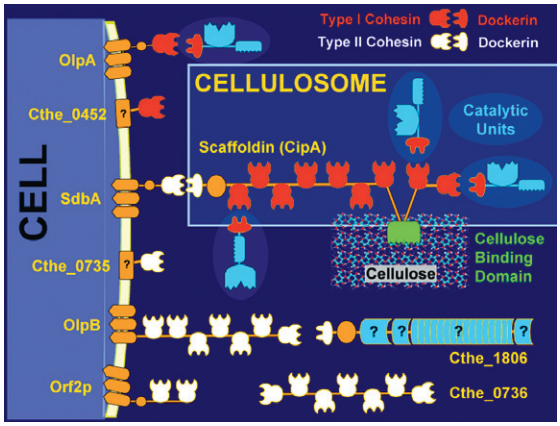
M. D. Ana, D. C. Carneiro, B. T. Airey, Z. Chong-Bin, L. Lu, E. J. Chesler, K. M. Erikson, and R. D. Blakely. "Functional coding variation in recombinant inbred mouse lines reveals novel serotonin transporter-associated phenotype," **Proceedings of the National Academy of Science** 106: 2047–2052 (2009).

Research Highlights

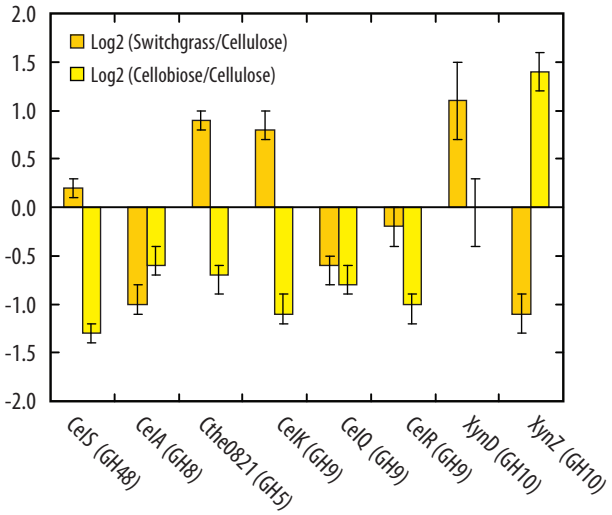
First proteomic study of *Clostridium thermocellum*

Scientists at the ORNL BioEnergy Science Center are employing systems biology approaches to understanding the conversion of cellulosic biomass to ethanol by the cellulolytic microorganism *Clostridium thermocellum*. For lignocellulosic ethanol production to be economically feasible and sustainable, robust microorganisms are needed that can efficiently degrade and convert plant biomass to ethanol. The anaerobic thermophilic bacterium *C. thermocellum* is a good candidate microorganism for biofuel production and can achieve efficient cellulose hydrolysis using multiprotein extracellular enzymatic complexes, or cellulosomes.

Bioscientists at ORNL recently completed the first proteomic study of this biomass-degrading enzyme system under real-world conditions using heterogeneous, natural lignocellulosic material, namely, pretreated switchgrass. They discovered that the relative composition of different carbohydrate active enzymes in the *C. thermocellum* cellulosome changes depending on the growth substrate. The study also identified and experimentally verified 16 "new" cellulosome components in *C. thermocellum* not previously detected in studies using model substrates. These insights provide building blocks for constructing designer cellulosomes with tailored enzyme composition for industrial ethanol production. To date, this study provides the most comprehensive comparison of cellulosomal compositional changes in *C. thermocellum* in response to different carbon sources. Such studies are vital to engineering a strain that is best suited to grow on specific substrates of interest.



Simplified schematic representation of Clostridium thermocellum *cellulosomal architecture. CipA is the backbone scaffoldin protein containing nine Type I cohesins and can accommodate up to nine Type I dockerin-bearing catalytic units. CipA also contains a Type II dockerin for cell-surface attachment via anchor proteins with Type II cohesins (e.g., SdbA, OlpB, Orf2p). CipA also has a cellulose binding domain for attachment to crystalline cellulose.*



Cellulosome compositional changes in response to carbon substrate. Plot illustrates changes in levels of selected key carbohydrate active enzymes in C. thermocellum *cellulosome during growth on pretreated switchgrass or the disaccharide, cellobiose, relative to growth on crystalline cellulose.*

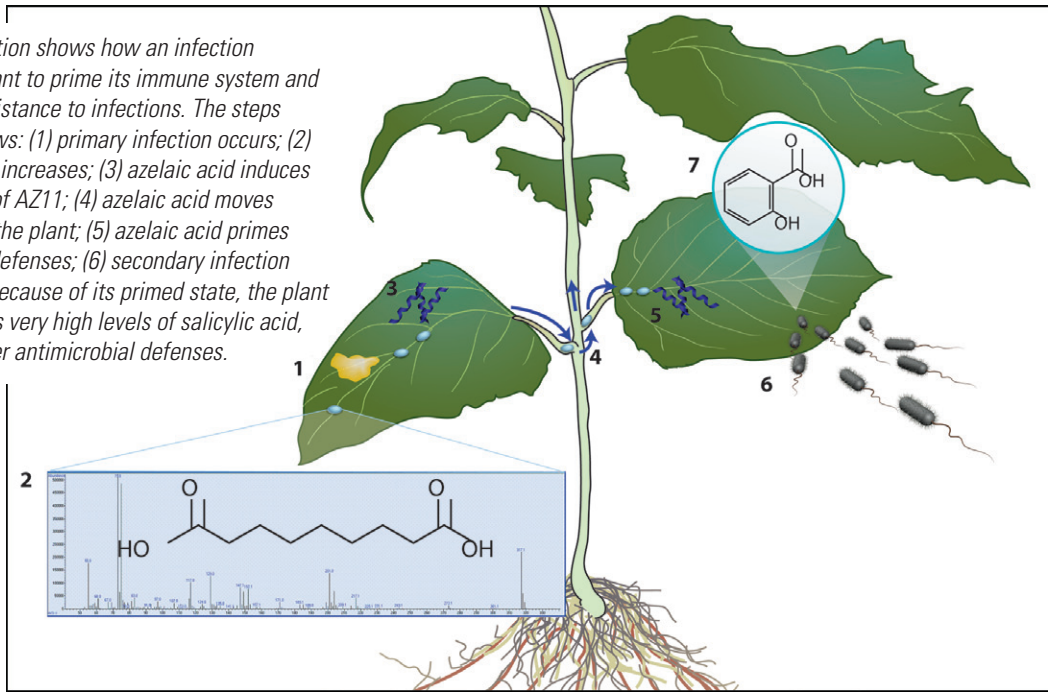
B. Raman, C. Pan, G. B. Hurst, M. Rodriguez, Jr., C. K. McKeown, P. K. Lankford, N. F. Samatova, and J. R. Mielenz. "Impact of pretreated switchgrass and biomass carbohydrates on *Clostridium thermocellum* ATCC 27405 cellulosome composition: A quantitative proteomic analysis," **PLoS ONE** 4(4): e5271 (April 2009), DOI:10.1371/journal.pone.0005271.

Research Highlights

Researchers discover primer to plant defense system

Researchers at Oak Ridge National Laboratory and the University of Chicago have discovered a key component that plays a critical role in priming a plant's immune response system.

Using *Arabidopsis*, a small flowering plant related to cabbage and mustard that is frequently used as a model for studying higher plants, they found that exposure to a bacterial pathogen caused the level of azelaic acid in this plant to increase significantly. A persistent mass spectral signature that appeared after *Arabidopsis* was exposed to the pathogen led to the initial discovery. This signature matched a pattern in a database of mass spectral signatures of plant metabolites. A number of other novel signatures were evident as well and may be the subject of future studies.



This illustration shows how an infection causes a plant to prime its immune system and improve resistance to infections. The steps are as follows: (1) primary infection occurs; (2) azelaic acid increases; (3) azelaic acid induces production of AZ11; (4) azelaic acid moves throughout the plant; (5) azelaic acid primes the plant's defenses; (6) secondary infection occurs; (7) because of its primed state, the plant accumulates very high levels of salicylic acid, which trigger antimicrobial defenses.

Through a process involving a very complex network of responses, the infected plant produces higher levels of azelaic acid, which stimulate the production of AZI1, a protein the researchers found to be essential for systemic plant immunity. As azelaic acid moves through the plant, it bolsters the plant's immune response system so that it can respond quickly and effectively to infection. Through this process, the plant also accumulates very high levels of the defense signal salicylic acid, which helps inhibit the progression of secondary infections.

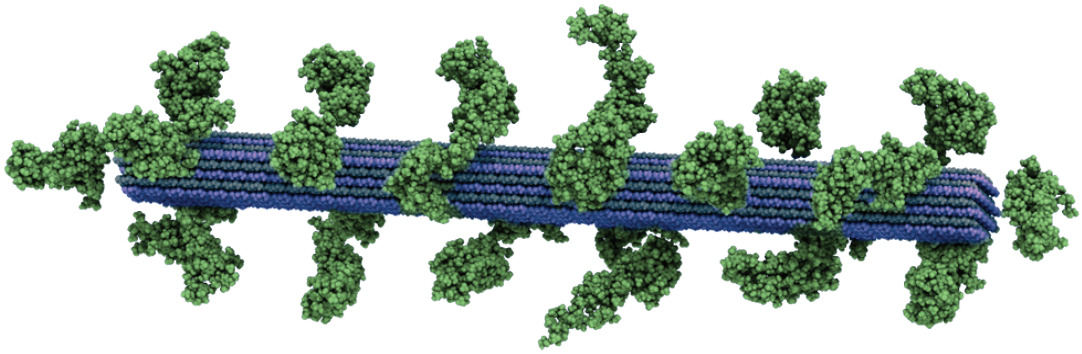
By identifying a compound that primes a plant's immune system, these researchers may be on their way to developing disease-resistant plants. Better understanding of the mechanisms by which exposure to pathogenic microbes can increase a plant's overall immunity to infection will prove useful in preventing disease in crops and other plants and in generating plants that by their very nature are more disease resistant.

H. W. Jung, T. J. Tschaplinski, L. Wang, J. Glazebrook, and J. T. Greenberg. "Priming in systemic plant immunity," **Science** 324(5923): 89–91 (April 2009), DOI: 10.1126/science.1170025.

Research Highlights

Computational modeling of lignocellulose

ORNL's supercomputers have been employed to examine the structure of lignocellulosic biomass, a potentially abundant and cheap source of sugar for industrial biofuel production. Lignocellulose is a complex material comprised mainly of cellulose, lignin, and hemicellulose. The overarching aim of this project is to build computational models of plant cell wall polymers—such as cellulose, lignin, and hemicellulose—and combine them toward a realistic model of lignocellulose. Molecular simulation complements experiments in obtaining an understanding of the structure, dynamics, and energetics of lignocellulose, providing insight as to the physical origin of biomass recalcitrance, its natural resistance against enzymatic deconstruction.



Atomic-detail model of cellulose (blue) and lignin molecules (green)

The complexity of biomass makes the construction of such a realistic model a challenging task. However, an integrated effort combining experiments at various BioEnergy Science Center sites (NREL and UGA) and the immense computational power available with ORNL petascale computers have made possible the simulation of preliminary atomic-detailed lignocellulose systems. This year scientists at ORNL have focused on building models using experimental input on the average chemical composition of softwood lignin. The information used was the unit and linkage composition and the fact that, despite containing chiral centers, lignin is optically not active. A very large atomistic model of lignin and cellulose comprising 3.3 million atoms was thus constructed and simulated on Jaguar, ORNL's supercomputer.

The ORNL group has devised a new strategy on how to best utilize petaflop supercomputers, such as Jaguar, to tackle lignocellulose simulation. Generally, there is an inherent difficulty in scaling molecular dynamics simulation (the method we are using) to many-thousand computer processors. This difficulty arises from the need to calculate the electrostatic interactions between millions of atoms. The proposed strategy is to use the Reaction Field (RF) method to compute these interactions. The recently published work demonstrates that the use of the RF is accompanied by a two-fold speedup of the simulation of lignocellulose, while not compromising the accuracy of the calculation.

L. Petridis, J. Xu, M. Crowley, J. C. Smith, and X. Cheng. "Atomistic simulation of lignocellulosic biomass and associated cellulosomal protein complexes biofuels," **ACS Symposium Series** (submitted).

R. Schulz, B. Lindner, L. Petridis, and J. C. Smith. "Scaling of Multimillion Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer," **J. Chem. Theory Comput.** 5(10): 2798–2808 (2009).

Research Highlights

Microarray-based genetic mapping in a genetically diverse plant species

Sugar release from native biomass during biochemical conversion is the single most restrictive factor in the development of a viable bioenergy industry for the production of transportation fuels. Discovering the genes that control cell wall composition and therefore sugar release is a challenging and complicated task. Various genetics and genomics tools can be applied to narrow a candidate gene list to those genes that may be directly related to sugar release.

Microarrays represent a powerful tool for genome-wide analyses of gene expression, allowing us to determine which genes are on during cell wall development. Microarrays can also be applied to genetic analysis of segregating populations by genotyping thousands of loci in a single assay, facilitating the identification of genomic intervals that contain genes that control the measured phenotypes. Although microarray-based genotyping approaches have been successfully applied in yeast and several inbred plant species, their power has not been proven in an outcrossing species with extensive genetic diversity such as *Populus*.

A team of scientists that included Tongming Yin and Gerald Tuskan of the Environmental Sciences Division recently reported on a method for high-throughput microarray-based genotyping in *Populus* using a pseudo-backcross progeny of 154 individuals of *P. trichocarpa* and *P. deltoides* analyzed with long-oligonucleotide in situ–synthesized microarray probes. The analysis resulted in high-confidence genotypes for 719 single-feature polymorphism (SFP) and 1014 gene expression marker (GEM) candidates. A high-density genetic map, comprising over 600 SFPs, GEMs, and SSRs, was constructed using these genotypes and an established microsatellite (SSR) framework map. The abundant gene-based markers allowed the location of over 35 million base pairs of a previously unplaced whole-genome shotgun (WGS) scaffold sequence to putative locations in the *Populus* genome. Their placement was verified with independently mapped SSRs, demonstrating the previously unutilized power that high-density genotyping can provide in the context of map-based WGS sequence reassembly.

The continued improvement of the *Populus* genome assembly will likewise improve the ability to conduct positional cloning of candidate genes related to cell wall formation, and at the same time facilitate microarray-based genotyping in a highly heterozygous population.

D. R. Drost, E. Novaes, C. Boaventura-Novaes, C. I. Benedict, R. S. Brown, T. Yin, G. A. Tuskan, and M. Kirst. "A microarray-based genotyping and genetic mapping approach for highly heterozygous outcrossing species enables localization of a large fraction of the unassembled *Populus trichocarpa* genome sequence," **The Plant Journal** 58: 1054–1067 (2009), DOI: 10.1111/j.1365-313X.2009.03828.x.

High-yield production of hydrogen from cellulosic materials and water

Carbon-neutral hydrogen gas is expected to be an important energy carrier in the future, particularly for powering vehicles. Hydrogen gas can be produced from many hydrogen-containing compounds, such as natural gas and water, but low-cost methods of producing hydrogen from renewably energy sources are needed.

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A research team including several members of the Biosciences Division is investigating ways of producing hydrogen at high yields from lignocellulosic biomass and water. A paper published in *ChemSusChem* detailing their results was among the journal's most cited papers of 2008–2009.

The goal of the effort was to produce hydrogen at high efficiency from a mixture of cellulosic materials and water. A novel synthetic enzymatic pathway was designed that employed a "cocktail" of 13 enzyme catalysts. The pathway included five modules that began by converting cellobiose to a form of glucose and ended with the generation of hydrogen from NADPH (nicotinamide adenine dinucleotide phosphate) at 93.1% efficiency. Hydrogen was also produced from the larger carbohydrate cellopentaose at 68% efficiency.

Thermodynamic analysis of the reaction indicated that it was spontaneous (when the reaction temperature was greater than 0°C) and endothermic (absorbing heat). It appears to be the first chemical reaction that can absorb ambient heat and convert it into usable chemical energy; that is, it is the first in which the ratio of energy output to energy input is greater than 1. Spontaneous endothermic chemical reactions are rare, but not unknown.

The spontaneous reactions catalyzed by enzyme cocktails display some unique features: a low-temperature reaction that absorbs low-temperature heat to produce hydrogen, a high hydrogen yield in a batch reaction, and a roughly eight-fold improvement in hydrogen production rate compared with previous efforts.

X. Ye, Y. Wang, R. C. Hopkins, M. W. W. Adams, B. R. Evans, J. R. Mielenz, and Y.-H. P. Zhang. "Spontaneous high-yield production of hydrogen from cellulosic materials and water catalyzed by enzyme cocktails," **ChemSusChem** 2(2): 149–152 (2009), DOI: 10.1002/cssc.200900017.

High levels of oxygen lead to decreased *Z. mobilis* ethanol productivity and inhibitor buildup

ORNL researchers have shown that high oxygen concentrations present during *Z. mobilis* fermentations negatively influence fermentation performance. The maximum specific growth rates were not dramatically different between aerobic and anaerobic conditions, yet oxygen did affect the cell physiology in such a way that metabolic by-products built up, which ultimately led to greater gene expression differences. Through these fundamental studies, ORNL scientists were able to identify a global regulator gene that was important for tolerance and survival of *Z. mobilis* and *S. cerevisiae* in response to several classes of lignocellulosic pretreatment inhibitors. A patent application (one of two for this project) and manuscript have been submitted describing these follow-on studies.

In this study, several different types of analyses were used to study the transcriptomic and metabolomic profiles for ZM4 aerobic and anaerobic fermentations. These analyses included microarray, high-performance liquid chromatography (HPLC), gas chromatography (GC), and gas chromatography–mass spectrometry (GC-MS). In the absence of oxygen, the ZM4 strain of *Z. mobilis* consumed glucose more rapidly, had a higher growth rate, and produced primarily ethanol. Greater amounts of other end products such as acetate, lactate, and acetoin were detected

Research Highlights

under aerobic conditions, and at 26 h there was only 1.7% of the amount of ethanol present aerobically as there was anaerobically. In the early exponential growth phase, significant differences in gene expression were not observed between aerobic and anaerobic conditions via microarray analysis. HPLC and GC analyses revealed minor differences in extracellular metabolite profiles at the corresponding early exponential-phase time point. Differences in extracellular metabolite profiles between conditions became greater as the fermentations progressed. Under anaerobic conditions relative to aerobic conditions, GC-MS analysis of stationary-phase intracellular metabolites indicated that ZM4 contained lower levels of amino acids such as alanine, valine, and lysine, and other metabolites like lactate, ribitol, and 4-hydroxybutanoate. Stationary-phase microarray analysis revealed that 166 genes were significantly differentially expressed by more than two-fold. Transcripts for Entner-Doudoroff (ED) pathway genes (*glk*, *zwf*, *pgl*, *pgk*, and *eno*) and gene *pdc*, encoding a key enzyme leading to ethanol production, were at least 30 times more abundant under anaerobic conditions in the stationary phase based on real-time quantitative-PCR results. Differentially expressed ZM4 genes predicted by The Institute for Genomic Research (TIGR) were also identified that were not predicted in the primary annotation, which led to a comprehensive reannotation of the ZM4 genome.

S. Yang and S. D. Brown. Microorganisms having enhanced tolerance to inhibitors and stress. Provisional Patent application, No. 61/184,961, 2009.

S. Yang, K. M. Pappas, L. J. Hauser, M. L. Land, G.-L. Chen, G. B. Hurst, C. Pan, V. Kouvelis, M. Typas, D. A. Pelletier, D. M. Klingeman, Y.-J. Chang, N. F. Samatova, and S. D. Brown. "Improved genome annotation for *Zymomonas mobilis*," **Nat. Biotechnol.** 27: 893–894 (2009).

S. Yang, D. A. Pelletier, T.-Y. S. Lu, and S. D. Brown. "The *Zymomonas mobilis* regulator Hfq and related *Saccharomyces cerevisiae* proteins contribute to tolerance against multiple lignocellulosic pretreatment inhibitors," **BMC Microbiol.**, submitted October 22, 2009.

S. Yang, T. J. Tschaplinski, N. L. Engle, S. L. Carroll, S. L. Martin, B. H. Davison, A. V. Palumbo, M. Rodriguez, Jr., and S. D. Brown. "Transcriptomic and metabolomic profiling of Zymomonas mobilis during aerobic and anaerobic fermentations,"**BMC Genomics** 10: 34 (January 2009), http://www.biomedcentral.com/1471-2164/10/34, DOI: 10.1186/1471-2164-10-34.

Awards & Achievements

Wilbanks

Wilbanks receives Presidential Achievement Award from the Association of American Geographers

Tom Wilbanks of the Environmental Sciences Division, a social scientist and researcher on the human dimensions of climate change, has been recognized by the Association of American Geographers (AAG) for his service to geography and the general scientific community.

Wilbanks, a UT-Battelle Corporate Fellow whose research career spans four decades, received the AAG's Presidential Achievement Award last March at the association's annual meeting from AAG Past President Thomas J. Baerwald, who selected him for the honor. The AAG Presidential Achievement Award was established in 2004 to recognize individuals who have made long-standing and distinguished contributions to the discipline of geography.

Efroymson

Wilbanks specializes in applying geographic, social science, and technological knowledge and perspectives to sustainable development issues, particularly in the areas of solving energy challenges in developing countries and understanding responses to climate change concerns.

Efroymson and Hanson elected Fellows of the American Association for the Advancement of Science

Rebecca Efroymson and Paul Hanson, both of the Environmental Sciences Division, were among the 486 individuals to be elected Fellows of the American Association for the Advancement of Science (AAAS) at the 2009 Annual Meeting held last February in Chicago. Election to the rank of Fellow is the highest honor bestowed by the American Association for the Advancement of Science (AAAS), which is the world's largest general scientific society and publishes the journal *Science*. The society strives to advance science through initiatives in science policy, international programs, and science education.

Hanson

Rebecca was recognized for her important contributions to the science and practice of ecological risk assessment. She has performed numerous ecological risk assessments for contaminated sites, including the burial grounds, ponds, streams, and watersheds on the Oak Ridge Reservation. Her research evaluating risk to plants, soil invertebrates, and microbial processes led to the development of assessment support tools including bioaccumulation models and ecotoxicity benchmarks.

Paul was cited for his distinguished contributions to research on carbon cycling in terrestrial ecosystems and scientific leadership in the field of forest response to environmental change. He is group leader of Ecosystem Science and Terrestrial Water-Carbon Cycles groups in the Environmental Sciences Division and has

Awards & Achievements

published many articles on forest carbon, water, and nutrient cycling. Paul also serves as subject editor for the journal *Global Change Biology*, a forum and focus for biological research on global environmental change.

Russell, former Mammalian Genetics and Genomics Director, receives Lifetime Achievement Award from the YWCA

Russell

Liane Russell was honored by the Knoxville YWCA with a Lifetime Achievement Award at a ceremony celebrating the 25th anniversary of their awards night last August. Liane was recognized for her rich legacy of scientific achievements and community activism. She continues to publish work performed at ORNL over the past 50 years and provides valuable insight to the DOE Low-Dose Radiation program.

Gu receives ESTCP Award

Gu

Baohua Gu of the Environmental Sciences Division and a team of other scientists from Shaw Environmental, the U.S. Geological Survey, and University of Illinois–Chicago were named winners of the Project-of-the-Year Award by the Environmental Security Technology Certification Program (ESTCP) of the U.S. Department of Defense. Their project was aimed at differentiating various natural and anthropogenic sources of perchlorate and their formation mechanisms through the application of oxygen and chlorine stable isotope analyses. Perchlorate, the subject of their investigation, is a human toxin that occurs both naturally and anthropogenically in groundwater and surface water and has been widely used in explosives, rocket propellants, and pyrotechnics.

Previous research on perchlorate conducted by Gu and his colleagues at ORNL earned them an R&D100 award and served as the basis for the project. Their earlier work enabled the isolation and recovery of trace quantities of pure perchlorate crystals from complex environmental matrices.

Due to the widespread use and occurrence of both natural and anthropogenic perchlorate in the environment, this research has resulted in far-reaching ramifications, ranging from public health issues to liabilities that could be imposed by environmental cleanup needs. Details of this work are provided in H. Bao and B. Gu, "Natural perchlorate has its unique oxygen isotope signature," *Environ Sci. Technol.* 38:5073–5077 (2004).

Awards & Achievements

McGinn

McGinn awarded Bronze Medal from the U.S. Environmental Protection Agency

Wilson McGinn of the Environmental Sciences Division received a Bronze Medal in recognition of his significant improvement to the risk-based concentration screening tables. His new table, which is available on the Internet, provides environmental professionals and the public with a state-of-the-art resource for evaluating environmental contamination. His medal was presented to him at the Office of Solid Waste and Emergency Response awards ceremony that was held last June.

Mielenz co-chairs biotechnology symposium

Jonathan Mielenz of the Biosciences Division served as a co-chairman of the 2009 Symposium on Biotechnology for Fuels and Chemicals. The focus of this year's symposium was development and deployment of renewable fuels and chemicals technologies.

Mielenz

BioEnergy Science Center highlights

At the ORNL BioEnergy Science Center, scientists are developing methods of producing biofuels from a variety of nonfood plants rich in cellulose, such as switchgrass and poplar trees. Their research involves seeking way to modify plant cell walls, which could reduce their resistance to breakdown and thus decrease or eliminate the need for costly chemical pretreatments that are currently being used. Consolidated bioprocessing, another area of their research, involves the use of a single microorganism or group of organisms to break down plant matter, which would allow biomass to be converted to biofuels through a one-step process.

Major accomplishments of the center this year included 84 scientific publications and 16 invention disclosures. The staff gave more than 211 scientific presentations and over 92 presentations to stakeholders (including members of Congress, Secretaries, Undersecretaries, and businesses). The staff also conducted 24 workshops and gave over 70 television, radio, and print interviews.

Davison

Davison named BER Genomics Chief Scientist and to the advisory panel for Canada NSERC Bioconversion Network

Brian Davison, systems biology chief scientist in the Biosciences Division, was named chief scientist of the Genomic Science research program of the Office of Biological and Environmental Research. The focus of this program is on developing technologies to understand and use the diverse capabilities of plants and microbes

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for innovative solutions to DOE energy and environmental mission challenges. Brian was also named to the advisory panel of the Natural Sciences and Engineering Research Council of Canada (NSERC) Bioconversion Network. The goal of this Canadian R&D network is to develop energy efficient, commercially viable, and environmentally sustainable biomass conversion processes that generate ethanol and high-value co-products.

Mulholland

Mulholland named a Fellow of the American Geophysical Union

Pat Mulholland of the Environmental Sciences Division was named a Fellow of the American Geophysical Union (AGU). The AGU is a worldwide association of scientists and lay public whose mission is to advance understanding of geophysical science for the benefit of humanity. Pat was recognized "for his seminal advances in the biogeochemistry and hydrology of stream and river ecosystems" during the AGU Honors Ceremony at the 2009 AGU Joint Assembly, held last May in Toronto, Canada. Each year only one Fellow is selected from every 1000 members of AGU.

Yang

Yang article named a "highly accessed paper" by *BMC Genomics*

A journal article prepared by lead author Shihui Yang and coauthors Timothy Tschaplinski, Nancy Engle, Sue Carroll, Brian Davison, Anthony Palumbo, Miguel Rodriguez, and Steven Brown of the Biosciences Division was named a "highly accessed paper" by *BMC Genomics*. The article, "Transcriptomic and metabolomic profiling of *Zymomonas mobilis* during aerobic and anaerobic fermentations," *BMC Genomics* 10:34 (2009), was given this designation based on the rapid and significant number of times it was accessed after its publication. Their study provides insights into transcriptomic and metabolic profiles of the model ethanogenic bacterium *Z. mobilis* during aerobic and anaerobic fermentation under controlled fermentation conditions for the first time. A range of genes that could be targeted for deletion to better understand *Z. mobilis* physiology and coordinate regulation is identified. A number of genes that were not originally annotated as coding sequences when the first *Z. mobilis* genome sequence was published are also identified.

Bader

Bader and Hanson testify before Congress on climate change

Dave Bader, manager of the ORNL Climate Change Research Program, and Paul Hanson, chief scientist for the DOE Ecosystem Research Program and an ORNL distinguished scientist, were invited to speak to the Energy and Environment Subcommittee of the House Science and Technology Committee. They discussed

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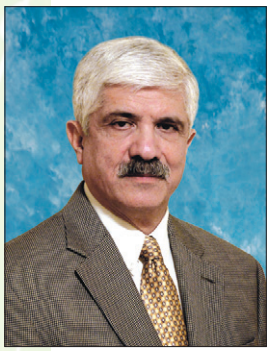
the importance of the National Environmental Research Parks (NERPs) to studies of the carbon cycle in local ecosystems. Such studies include manipulations in temperatures, precipitation, nutrient content, and carbon dioxide levels to examine the role of ecosystems in mediating emissions of greenhouse gases and how climate change may impact the exchange of carbon between the atmosphere and the earth. They also explained the importance of field measurements and experiments for validating and improving the accuracy of computational climate models, as well as providing insights into ways the models can be modified to better reflect observations of field conditions.



Sokhansanj

Shahab Sokhansanj elected a Fellow of the American Society of Agricultural and Biological Engineers and receives 2009 Maple Leaf Award, Canadian Society of BioEngineering

The American Society of Agricultural and Biological Engineers (ASABE) has named Shahab Sokhansanj of the Environmental Sciences Division to its 2009 class of ASABE Fellows. The ASABE is a scientific and educational organization dedicated to the advancement of engineering applicable to agricultural, food, and biological systems. He was selected for the honor in recognition of his outstanding accomplishments in agricultural engineering through training of postgraduate students, his innovative research in post-harvest engineering, and his exemplary service to ASABE.

The Canadian Society of BioEngineering (CSBE/SCGAB) also honored Shahab with its 2009 Maple Leaf Award. It is the highest award given to members of the society who have distinguished themselves as leaders in the profession and in recognition of their personal qualities, society activities, and professional abilities.

Sorensens receive Independent Film and Video Award

John Sorensen and Barbara Vogt Sorensen were the recipients of two Aurora Awards, an independent film and video competition, for their videos "Animals in Emergencies" and "Operations Level Training: A Refresher for Responders," which were prepared for the Chemical Stockpile Emergency Preparedness Program (CSEPP) of DHS-FEMA. The animal video is intended to help pet and livestock owners incorporate protective actions for animals into emergency plans and to assist in planning for evacuation or sheltering animals in emergencies. Both English and Spanish versions were produced. The Director of FEMA sent copies to every U.S. representative and senator to demonstrate the timeliness of the product. The responder video provides operations-level refresher training as specified in CFR 29 1910.120 for first responders involved in hazardous material emergencies. The

Awards & Achievements

Aurora Awards is an international competition designed to recognize excellence in the film and video industries. It specifically targets products, programs, and commercials that would not normally have the opportunity to compete on a national level, by focusing on non-national commercials, regional or special-interest entertainment, and corporate-sponsored film and video.

New Center for BioEnergy Sustainability at ORNL

The Center for BioEnergy Sustainability (CBES) was established by ORNL to bring unique skills and technical expertise to sustainability problems of national and global concern regarding the environmental impacts and sustainability of biomass production and its conversion to biofuels and bio-based products. The mission of this center is to use science and analysis to understand the sustainability (environmental, economic, and social) of current and potential future bioenergy production and distribution; to identify approaches to enhance bioenergy sustainability; and to serve as an independent source of highest quality data and analyses for bioenergy stakeholders and decision-makers. CBES creates opportunities to bring ORNL scientists and other stakeholders together to identify research opportunities and strategies to target specific goals through a collaborative approach. Monthly forums hosted by CBES provide an opportunity for sharing information through the presentation of current research activities and challenges. CBES has hosted workshops and plans to host a minimum of two workshops per year. In May, CBES organized a workshop on "Land-Use Change and Bioenergy" at which leaders in global land-use-change modeling and experts on the land-cover and land-use data sets were assembled and developed strategic research plans to fill key gaps and improve science-based approaches for measuring the impacts of biofuel policies and programs on land use and related emissions. CBES also hosted an informal workshop for ORNL and the U.S. Environmental Protection Agency on "Sustainability of Bioenergy Systems: Cradle to Grave" in September. This workshop created opportunities to present key issues of bioenergy sustainability and discuss work that is ongoing to address these issues based on a systems perspective and to identify questions that lead toward a workable definition of bioenergy sustainability. A third workshop, "A Watershed Perspective on Bioenergy Sustainability," will be held in February 2010. Additional information is available at the CBES website at http://www.ornl.gov/sci/besd/cbes/.

Awards & Achievements

Essential Science Indicators "hot paper"

A journal article by lead author Wei-Min Wu of Stanford University and coauthors Jack Carley, Terry Gentry, Tonia Mehlhorn, Hui Yan, Sue Carroll, Molly Pace, Baohua Gu, David Watson, Jizhong Zhou, and Philip Jardine of the Environmental Sciences Division was named a "hot paper" by Essential Science Indicators. The article, "Pilot-Scale in Situ Bioremediation of Uranium in a Highly Contaminated Aquifer. 2. Reduction of U(VI) and Geochemical Control of U(VI) Bioavailability," appeared in *Environmental Science & Technology* 40(12), 3986–3995 (2006). A hot paper is a designation used by Essential Science Indicators to recognize papers that are cited very frequently and soon after their publication.

Cheng

Cheng wins SERDP Project-of-the-Year Award

Meng-Dawn Cheng of the Environmental Sciences Division was named the winner of the Project-of-the-Year Award by the Strategic Environmental Research and Development Program (SERDP) of the U.S. Department of Defense for his development of a comprehensive program for measuring emissions from military aircraft.

As military jet air service needed for transporting of cargo and soldiers continues to increase, the levels of aircraft fuel and emissions will likewise increase, which can be harmful to human health and local and regional air quality and visibility. The emission-characterization program developed by Cheng and his team has made available to the military state-of-the-art measurement techniques and instruments for measuring military aircraft emissions.

SERDP was established as a partnership among the Department of Defense, the Department of Energy, and the Environmental Protection Agency to address the highest priority issues facing the Army, Navy, Air Force, and Marines.

Wilkerson

Wilkerson receives Presidential Citation from the American Society of Agricultural and Biological Engineers

Erin Wilkerson of the Environmental Sciences Division received a Presidential Citation from the American Society of Agricultural and Biological Engineers (ASABE) for her leadership in coordinating the technical program and organizing volunteers for the first-ever Bioenergy Engineering Conference held October 11–14 in Bellevue, Washington. The citation on her awards plaque reads as follows: "For dedication to ASABE and leadership in the development of the Bioenergy Engineering Conference and continuous efforts put forth to advance the objectives of the Society."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