Oak Ridge National Laboratory

REVIEW

• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

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The Resurgence of Bioenergy

A Solution to Energy Security

The Business of Biomass

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Jonathan Mielenz, leader of the Bioconversion Science and Technology Group in ORNL's Biosciences Division, is studying a microbe that could prove more cost effective than current methods in transforming cellulose from sources such as switchgrass and poplar trees into ethanol.

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Reinhold Mann, Associate Laboratory Director for Biological and Environmental Sciences at Oak Ridge National Laboratory, is leading ORNL research efforts to produce biofuels from poplar trees and switchgrass.

A TRANSFORMATIONAL CHANGE

In 1908 Henry Ford constructed an ethanol fermentation plant in Atchison, Kansas, designed to fuel the first generation of his newest car, the Model T. The investment represented Ford's belief that ethanol would be the primary fuel for the emerging American automobile. In this instance, Ford's prediction was wrong. By the close of World War II, the discovery of seemingly unlimited supplies of oil had greatly reduced the price of gasoline and diesel fuel, to the point that ethanol made from biomass essentially disappeared from the American market.

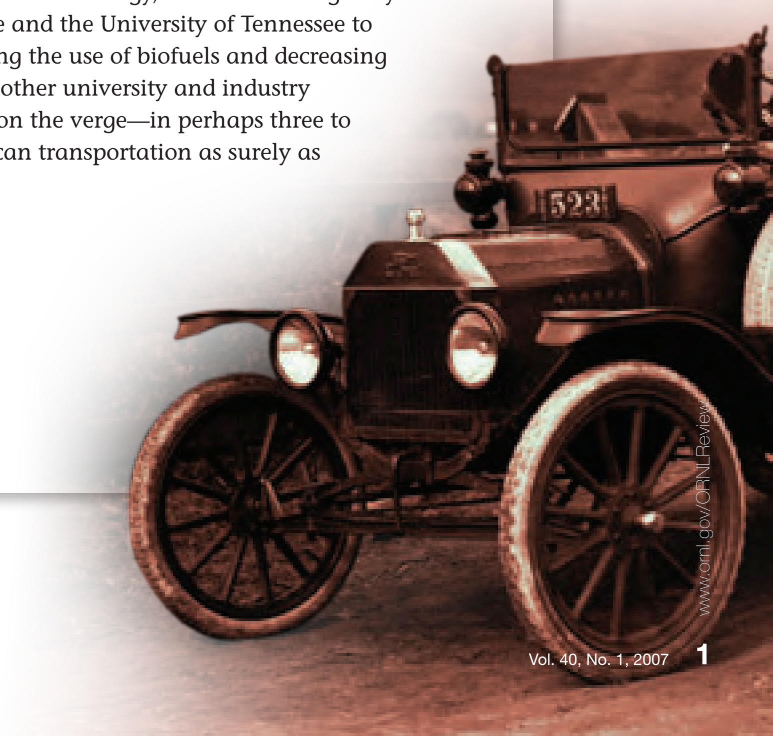
Nearly a century later, a combination of political, financial and environmental factors has rekindled America's interest in Ford's original belief that biofuels can be a major component of the fuel needed to run the nation's transportation system. In a world market now under growing pressure from diminishing reserves and increasing demand, the cost of petroleum is reaching levels unimaginable only a decade ago. Across the continents of Africa and Southern Asia, prolonged political instability threatens fragile oil supply lines. At home, the annual consumption of more than 300 billion gallons of fuel made from petroleum in combustion engines is a major contributor to unprecedented levels of greenhouse gas in Earth's atmosphere.

Led by the Department of Energy, America is moving toward a transformational change that includes the displacement of petroleum with carbon-neutral, renewable sources of transportation fuels. President George W. Bush has established a goal that by the year 2030 the equivalent of 30 percent of the gasoline used on U.S. highways will be replaced with biofuels. With biofuels accounting for only about three percent of current motor fuels consumption, the technological challenge is among the most daunting of the new century.

This issue of the *ORNL Review* is dedicated to the efforts of researchers at Oak Ridge National Laboratory to help develop transportation fuels from lignocellulosic biomass in a manner that is environmentally sustainable and cost competitive with petroleum. The work thus far is promising. ORNL is moving beyond conventional methods of producing ethanol from corn, using cutting-edge research to develop exciting new kinds of biofuels from crops such as switchgrass and poplar trees. Our effort is multi-faceted and cross-disciplinary, addressing the economic, environmental and agronomic issues associated with bioenergy production. Our research employs some of the most advanced analytical tools available, including the world's most powerful neutron scattering facilities and America's largest open-science, ultrascale computer. With these unique resources, we are coming closer each day to understanding plants with bioenergy crop potential, as well as microbes and microbial communities to process biomass into fuels and the molecular mechanisms and dynamics of biocatalysis.

As we undertake this challenge with the Department of Energy, we are encouraged by a commitment from both the Governor of Tennessee and the University of Tennessee to lend their resources in the common goal of increasing the use of biofuels and decreasing carbon emissions. Working together with these and other university and industry partners, we are increasingly confident that we are on the verge—in perhaps three to five years—of discoveries that will transform American transportation as surely as Henry Ford's Model T did more than a century ago.

Reinhold Mann
Associate Laboratory Director
Biological and Environmental Sciences



AMERICA RESPONDS

A renewed interest in bioenergy offers a solution to energy security.

Jerry Tuskan with a poplar seedling. He led an international consortium of researchers to sequence the genome of black cottonwood, or Populus tricho-carpa*, a hybrid poplar that shows promise as a bioenergy crop.*

The multi-lane, rush-hour collection of SUVs, sedans and trucks that choke the nation's highways, the incessant road construction projects that tease of faster routes to come, the suburban residential sprawl radiating from commercial urban centers, the acres of asphalt surrounding grocery stores and retail malls—all testify to the inextricable relationship between Americans and their automobiles.

Approximately 140 billion gallons of gasoline per year power this dependency, and the consequences of this addiction to America's economy and foreign policy are profound. While Americans consume 25 percent of the global oil supply, our nation

claims just 3 percent of the world's known reserves. This simple fact reveals the uncomfortable truth that 60 percent of U.S. transportation fuel flows from foreign sources.

Buried deep inside the earth, the energy storehouses bequeathed by the living things of previous millennia threaten to become increasingly costly under modern society's ever more voracious appetite for fossil fuel. The debate over the exhaustibility of these reserves is no longer over "if" but "when," as burgeoning Asian economies demand an increasing share of the world's finite petroleum supply. The uncertainty of access to remaining fossil resources, divided unevenly among a handful of countries with varying levels of political stability, poses what many regard as the greatest threat to America's national security since World War II.

The threat of global climate change, influenced in part by emissions from U.S. cars and trucks, has intensified the need for fossil fuel alternatives. In 2004, American vehicles pumped 1.9 billion metric tons of carbon dioxide into the air, a number that is expected to grow to 2.7 billion tons by 2030. In China, emissions from factories and homes have produced the world's worst concentration of urban smog. Similar trends worldwide, coupled with historic increases in the price of petroleum, create what many researchers and policymakers believe is the critical impetus needed to at last develop energy sources capable of providing affordable and sustainable supplies of fuel to power the convertibles and minivans of generations to come.

The promise of providing Americans a practical source of affordable fuel at the corner quick-stop may not lie underground. According to a growing number of scientists and government policy makers, the solution grows above it. Already, ethanol distilleries have tapped the nation's largest crop, corn, to displace 3 percent of the current gasoline supply. But even as corn-based ethanol plants spring up across the country, experts recognize that corn, like petroleum, has limitations as a source of fuel.

The untapped potential of biofuels—that is, gas or liquid fuels derived from plant material—grows in cellulosic biomass, the fibrous, woody matter that gives a plant resilience and shape and is generally found distasteful to animals and people.

The possibilities contained in stalks, trunks and leaves of some plants—notably switchgrass and poplar trees, which offer the quickest path to market because much of their genetic make-up and production potential is already known—have caught the attention of government, scientists and industry at the highest levels. Governors and state legislatures in New York, Illinois, Indiana, Iowa, California and Tennessee (see sidebar p.18) have committed millions of dollars into biofuel initiatives. Established companies such as Archer Daniels Midland and start-ups such as Iogen of Canada are exploring new ways to generate cellulose-based ethanol and building pilot plants. Virgin Airlines' owner Sir Richard Branson is investing substantial sums dedicated to groundbreaking research in renewable fuels. The financial potential found in renewable fuels is evidenced by increasing interest from the oil industry itself. British Petroleum—which recently adopted the moniker "Beyond Petroleum"—is establishing research partnerships and making substantial investments in renewable energy alternatives.

Perhaps the most significant endorsement for bioenergy came when President George W. Bush in his 2006 and 2007 State of the Union address as mentioned wood chips, switch grass and the potential of biomass-based fuel sources. Spurred in part by a report known as the "Billion Ton" study and developed primarily by researchers at Oak Ridge National Laboratory and co-released by the U.S. departments of Energy and Agriculture (see sidebar), the Administration has promised new funding for biofuels research. The President has set a goal of displacing 30 percent of current U.S. liquid transportation fuel consumption with biofuels by 2030. Biofuels will include primarily ethanol from wood and switchgrass but also biodiesel made from soybeans and waste oils collected from the food service industry.

This is not the first time bioenergy has been part of the national energy discussion. The energy crisis of the 1970s, with accompanying gasoline shortages and price spikes, motivated Washington to fund a number of alternative energy research programs in an attempt to harness the power of plant life. However, as gas prices retreated and availability was restored, attention and research funding switched to other priorities.

What may provide the current push for bioenergy with staying power to survive fluctuations in world oil prices, is that the more transient concerns of economics and the environment are no longer the dominant considerations of energy policy, says ORNL's Martin Keller. Keller recently left Diversa, a publicly traded enzyme development company, to become director of ORNL's Bioscience Division and help lead the Laboratory's accelerating bioenergy research initiatives.

"For the first time national security has emerged as a major driver toward bioenergy, Keller says. "Even climate change, as serious as it may be, is not a strong enough motivation to produce a fundamental change in the way Americans look at bioenergy. Much of our society views the future in terms of only one to two years. This mindset explains why many people do not put money into savings for retirement, which tells us that economics, at present, is also not a driver for bioenergy."

Keller believes that since Sept. 11, 2001, the nation's heightened awareness of national security threats has placed the bioenergy discussion in a new context and presents new opportunities for ORNL. Sixty-five years ago, similar threats to national security resulted in an extraordinary effort to develop an atomic weapon, made possible in large measure by scientific research in Oak Ridge. Today, the Laboratory, with a 25-year track record in biomass development and world-class capabilities in the biological, computational and materials sciences stands poised to address, in a different scientific arena, a major national security challenge.

"Addressing the energy issue is critical to sustaining our society and our freedom," Keller says. "We need to bring the energy deficit under control so our kids can enjoy the freedom we have now."

"We need to bring the energy deficit under control so our kids can enjoy the freedom we have now." *Martin Keller*

A molecular quest

The trees and grasses that hold great promise as future sources of fuel also present the greatest resistance. The lattice of cellulose, hemicellulose and lignin render plant cell walls resistant to breakage and the ravages of weather, insects and disease. They also serve as a barrier to transforming the plants into simpler sugars that can be processed into ethanol or other types of fuels and chemicals.

Methods exist to make ethanol from cellulose, says Jonathan Mielenz, who heads up ORNL's bioprocessing program. However, the process costs about $2.26 per gallon of ethanol—a price much higher than gasoline because ethanol typically is only 60 percent as efficient. A White House initiative calls for reduction of the cost of producing cellulosic ethanol to $1.07 per gallon by 2012.

"The technology for making cellulosic ethanol has been known for 30 years, but the challenge we have not yet solved is how to make the fuel economically competitive with gasoline," Mielenz says. "With fossil fuels, you just pump oil out of the ground, do some catalytic cracking and separations and get gasoline and petroleum chemicals. Even with transportation costs, it is still cheaper to import and refine oil into gasoline than to turn a coffee table into ethanol."

The steps of cellulosic bioprocessing include thermochemical pretreatment of plant matter to render cellulose and hemicellulose biopolymers more accessible to enzymatic breakdown into glucose and xylose sugars; application of enzymes called cellulases to break up the complex carbohydrates into simple sugars, and, finally, fermentation by microbes to transform the sugar into alcohol. The alcohol is purified through distillation to make ethanol for vehicular use. Byproducts of the process can be turned into valuable chemicals to replace petrochemicals as well as produce heat and electricity to bolster profitability of the plants. Biorefineries potentially could produce other forms of fuels for transportation and heating.

The secret to cracking the code of cheap cellulosic ethanol production, Mielenz and other scientists believe, will be found in probing the molecular mechanisms involved, identifying new and better bacteria and enzymes needed to improve the process and genetically manipulating them to do their jobs even more efficiently. Certain microbes, for example, show promise in replacing harsh and expensive chemicals and, perhaps, combining steps of the bioprocess. ORNL researchers are using microarray technology to determine particular genetic functions of *Clostridium thermocellum*, a microbe genetically engineered at Dartmouth College to take on the double duty of very rapidly hydrolyzing cellulose with its own cellulases and fermenting sugar to ethanol mixed with two acids.

Eventual success in large-scale ethanol production is linked to the creation of a new agricultural industry capable of growing approximately 1 billion tons of biomass needed to displace 30 percent of the nation's current consumption of liquid transportation fuels.

The "Billion Ton" study estimated that about 50 million acres could be employed in production of biomass products such as switch grass and poplar trees. These are two of the most likely candidates for early production of biofuel because of their broad adaptability, the ability to modify easily existing agriculture methods to produce them and their current readiness for production, enabled by a 25-year DOE biomass program managed at ORNL.

Bob Perlack is the lead author of the "Billion Ton" study, a report that quantifies the bioenergy potential of U.S. land resources and influenced federal policy.

In addition to looking at the economic and societal implications of creating such a large agri-industry from scratch, Laboratory researchers also are working to develop plants most ideal for growing and harvesting as bioenergy crops. ORNL plant geneticist Gerald Tuskan recently led a two-year effort to sequence the genome of black cottonwood, or *Populus trichocarpa*, a hybrid poplar that scientists are seeking to develop into a tree uniquely suited to the needs of the bioenergy business. With the complete genome sequence in hand, Tuskan and his colleagues hope to find and identify genes responsible for promoting fast growth, increased biomass production and other characteristics such as drought tolerance and resistance to disease. Potentially, genetics could also be used to create a tree with cellulose and hemicellulose that are less resistant to breakdown, reducing cost at the bioprocessing plant. Such genetic tools allow scientists to accelerate the kinds of selective breeding that typically takes place over centuries.

"Farmers have spent thousands and thousands of years domesticating tradi-

Martin Keller, director of ORNL's Biosciences Division, and Brian Davison, ORNL chief scientist for systems biology and biotechnology, are leading the Laboratory's bioenergy research efforts.

The Billion Ton Study

Many reports penned for the U.S. government sit on shelves and collect dust. But government officials have been repeatedly citing an ORNL study on the possibilities for growing and gathering biomass on American soil, making the report a potential collector's item.

In 2004 ORNL's Bob Perlack, Lynn Wright, Anthony Turhollow and Robin Graham began preparing a report for the Departments of Energy and Agriculture that addressed this question: Are the U.S. land resources capable of producing a sustainable supply of biomass sufficient to displace at least 30 percent of the country's current petroleum consumption? The answer given in the report published in April 2005 is yes. "Looking at just forestland and agricultural land," the ORNL authors wrote, "this study found over 1.3 billion dry tons per year of biomass potential—enough to produce biofuels to meet more than one-third of the current demand for transportation fuels."

The "Billion Ton" study, as it came to be called, had a transforming effect, nudging the federal government into a policy shift.

President George W. Bush mentioned the report in a speech he made on energy in May 2005. "A recent study by Oak Ridge

tional agriculture crops in an almost serendipitous way," Tuskan says. "We hope to use genomics and modern genetics to shorten that domestication period to just a few decades."

The big picture

The multidisciplinary systems strategy required to meet bioenergy's scientific challenges makes ORNL uniquely qualified to carry out such a project.

"The reason I came to Oak Ridge is because I saw that national labs can provide an environment that enables research across lots of disciplines," Keller says. "I feel strongly that the future of science needs interaction of disciplines to work on bigger problems. With bioenergy, our challenge is to find a creative way to understand data and develop models to understand how cells really work."

Such collaborative investigation involves not only biologists, ecologists and geneticists, but also researchers in the fields of computational simulation, materials, nanotechnology, engineering and physics. At ORNL, researchers utilize one of the world's most powerful supercomputers to model mechanisms by which bacterial and fungal cellulases break down and chemically process cellulose. At the Laboratory's newly opened Nanoscience Center, researchers Tim McKnight and Udaya Kalluri will use DNA-coated carbon nanofibers to test whether a suspect cellulose-synthesizing gene introduced into a single naked poplar cell builds a cell wall. Potential also exists to examine the properties of biological materials at the Laboratory's Spallation Neutron Source, a $1.4 billion new instrument that will reach full beam power in the next couple of years. At the University of Tennessee — one of ORNL's managing partners — microbiologists are working with electrical and chemical engineers to apply engineering principles to questions of how cells are regulated, evolve and can be manipulated.

"Potentially, one could envision integrating cells directly onto some type of nanostructure or material to carry out a bioprocess," says Gary Sayler, head of the Joint Institute of Biological Sciences, a partnership between ORNL and UT.

A more holistic approach to biology promises to bear fruit in the quest for new energy sources as well, says Brian Davison, chief scientist for systems biology and biotechnology at ORNL. "We are in the middle of the second wave of the biotechnology revolution. The first wave of the biological revolution was the ability to amplify and manipulate a gene," he says. "The second wave seeks to analyze and understand biological systems. The essence of systems biology is the intent to approach the whole organism or pathway or community as a system rather than a reductionist single gene or single enzyme or 'black box' organism."

ORNL's historic expertise is now bolstered by a strategy to employ rapid improvements in instrumentation and simulation needed to explore and process that information. "First, we intend to attack this problem aggressively," Davison says. "Second, we have strong capabilities in bioinformatics and computation. Third, we have historical strengths in biology, environment, plants and microbes and knowledge about their relevance to bioenergy."

Mark Downing, an ORNL agricultural economist, casts a likely historic effort in these terms: "Bioenergy is not the science, it is the result of doing good science. You get good science from superior work of a dozen different researchers, and that is what ORNL does best."—*Larisa Brass*

National Laboratory projected that biofuels such as ethanol and biodiesel could provide about a fifth of America's transportation fuel within 25 years," the President said in remarks at the Virginia Biodiesel Refinery at West Point, Va. Fast forward to the President's State of the Union address on January 31, 2006, when he proclaimed, "We'll also fund additional research in cutting-edge methods of producing ethanol, not just from corn, but from wood chips and stalks or switchgrass."

The "Biomass as Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply" report was an impetus for the 2006 DOE initiative to produce some 60 billion gallons of ethanol from biomass to replace 30 percent of the petroleum used for transportation fuel by 2030.

Jonathan Mielenz, leader of the Bioconversion Science and Technology Group in ORNL's Biosciences Division, says, "The Billion Ton study was a critical contribution because it provided evidence for the biomass ethanol and chemical industries that a real and substantial resource base could be potentially available from which to build their businesses. This knowledge gave decision makers in government and elsewhere credible arguments to support funding and policy decisions needed for a fledgling biorefinery industry."

Offering possible reasons for the report's success, Perlack says, "We chose to focus on biomass resources and avoid discussing policy and cost. We kept the study narrow and simple. And best of all, the report came out just when gasoline prices started their long climb." —*C. K.*

THE PEOPLE'S TREE

ORNL teams seek to make the poplar tree an affordable raw material for biofuels and bioproducts.

In the days of the Roman Empire, people met under trees with leaves that fluttered noisily in the slightest breeze. These trees came to be known as *arbor populi*, or "the people's tree." The poplar tree, also known as cottonwood and aspen, certainly stands up to the name.

For centuries, foresters have treasured black cottonwoods (*Populus trichocarpa*) because they can be sold for lumber, plywood and pulp for paper. Today, scientists also believe the species holds in its woody fibers the fuel needed to shift a significant segment of America's foreign oil dependency to local, renewable energy sources in the not-so-distant future.

When Oak Ridge National Laboratory managed the Bioenergy Feedstock Development Program for the Department of Energy from 1978 to 2001, the ORNL team chose to focus on the improvement and management of just a few "energy crops" rather than a multitude of grass and tree species. They selected switchgrass and two tree species—willow and poplar—for carbon sequestration and bioenergy studies.

Researchers gathered data on these rapidly growing plants and applied breeding techniques for crop improvement to increase plant productivity and the drought tolerance of these energy crops. Their study determined the best crop management practices, such as the minimum amount of water, fertilizer and pesticides needed as well as when and how often these should be applied.

Since the completion of the human genome sequencing project, DOE's Joint Genome Institute in California has been determining the order of DNA bases in hundreds of one-celled microorganisms. Three years ago, Stan Wullschleger, a plant physiologist and leader of plant molecular ecology research at ORNL, and plant geneticist Jerry Tuskan in Wullschleger's group proposed that a multinational partnership sequence the first tree genome.

Sequencing the *Populus* genome

"It is difficult to move forest biology forward by studying trees in a greenhouse or forest," Tuskan says. "We proposed to DOE that we could accelerate the development of bioenergy crops by sequencing the genome of the black cottonwood."

One way ORNL promoted the decoding of the hybrid poplar was through the formation of the International Populus Genome Consortium to support the effort. DOE provided funding for the project of sequencing the *Populus* genome, which was completed in less than two years by JGI and an ORNL team led by Tuskan. Tuskan then led a multinational team of 250 scientists from 34 nations in analyzing the genetic blueprint of the first tree genome. Tuskan worked closely with scientists at JGI and universities in the United States, Austria, Canada, Belgium, Finland, France, Germany and Sweden. The analysis of the complete sequence of the genome of a female black cottonwood tree that grew along the Nisqually River in Washington was published September 15, 2006, in *Science* magazine.

"We think we have captured most of the 45,500 genes on 19 chromosomes in the *Populus* genome," Tuskan says, pointing out that in comparison the human genome is now thought to have 22,000 to 28,000 genes on 23 chromosomes. *Populus* has 485 million DNA base pairs, making the tree four times larger than *Arabidopsis thaliana*, a mustard weed and the first plant to be sequenced.

"One of the four algorithms 'trained' to find genes in *Populus* was developed at ORNL," Tuskan adds. "Oak Ridge researchers annotated the sequence to predict the functions of genes, including those associated with stem growth, biomass production and other bioenergy-relevant abilities. Our task now is to use that information to accelerate the domestication of the poplar tree for biofuels and biomaterials development."

"The poplar genome project is a major step toward the day when the production of biofuels becomes a major element in the world's energy supply," says ORNL Director Jeff Wadsworth.

ORNL researchers are among the world's leaders in woody plant genomics, says Brian Davison, the Laboratory's chief scientist for systems biology and biotechnology. He explains that ORNL plant scientists have a unique opportunity to "design" poplars

for carbon sequestration and bioenergy. "The Lab's researchers have identified carbon partitioning genes and carbon allocation genes," he says. "These genes determine the relative amounts of carbon from atmospheric carbon dioxide that are stored in a tree's roots, trunk, branches and leaves."

Knowledge of the poplar's genetic code will enable plant geneticists to modify poplars to grow more wood and a higher fraction of cellulose and hemicellulose. Aboveground tree biomass is 26 percent lignin, 20 percent hemicellulose and 44 percent cellulose.

Tuskan's colleagues found 93 protein-coding genes associated with the production of cellulose, hemicellulose and lignin, the building blocks of the tree's cell walls. Enzymes can degrade cellulose and hemicellulose into sugars. These sugars, in turn, can be fermented into alcohol, which is distilled to yield fuel-quality ethanol.

Making cellulosic ethanol affordable

Now that researchers have learned how to make ethanol from cellulose, the next challenge is to make the process affordable for commercial use. To help lower the cost of converting cellulose from trees to ethanol, Tuskan and his ORNL colleagues are analyzing the *Populus* genome to identify genes that could be disabled or amplified to create a tree with more desirable traits. The researchers would like to increase the poplar's productivity and its ability to tolerate stresses such as drought and extremely cold weather, as well as resist attacks by insects and pathogens.

Accelerated domestication of the poplar tree is desirable to create a cost-effective feedstock plant tailored for economical ethanol production. Tuskan cites corn as an illustration. American cornfields today have 25,000 corn stems per acre. At the beginning of the 20th century, only 10,000 stems could be grown on an acre because the corn leaves extended laterally instead of vertically, as they do today.

"Older varieties of corn also have a phytochrome gene that allows the plant to detect light reflected from its neighbor," Tuskan says. "Plants grown too close together did not grow well. Through many decades of breeding and selection, the phytochrome gene in corn has been disabled so that the plant barely senses its neighbors."

Domestication of corn took a century. ORNL plant scientists seek to domesticate the poplar in 15 years. In five years they hope to produce trees with new properties, and within 10 years they plan to establish plantations of genetically modified poplars as energy crops in approved field tests.

For carbon sequestration, researchers have been genetically redesigning poplars to shuttle more carbon into the roots for long-term storage in the soil, slowing the buildup of climate-altering atmospheric carbon dioxide. For bioenergy, the goal is to disable or amplify poplar genes so that less carbon goes into stem height and branch growth and more carbon goes into the tree trunk's radial growth. By understanding how to manipulate bioenergy-relevant genes and molecular "dimmer" switches that turn protein-coding genes on and off or up and down, Tuskan's team hopes to produce managed tree systems with more biomass in the right places. Within the next three to five years, the ORNL researchers believe they can create a genetically modified poplar tree with a shorter, thicker trunk, or stem, and fewer branches.

Results from ORNL's bioenergy feedstock program indicate that an annual yield of 10 tons of wood per acre of poplars is both achievable and practical. "Our goal is to get 20 tons per acre per year of biomass from trees using less water and nutrients," says Tim Tschaplinski, an ORNL plant physiologist and biochemist. "We want these trees to be able to grow in most regions of the United States, even under drought conditions, and to be harvested in six to seven years.

"We hope to reconstruct the architecture of the hybrid poplar and accelerate its domestication," Tschaplinski adds. "The key features of a highly productive poplar include a narrow crown with fewer lower branches that crowd its neighbors and reduce productivity. We prefer more branching at the top of the tree's crown for the capture of light for photosynthesis. Crowns shed these upper branches after only a few years."

A shorter, broader tree with fewer branches is easier and cheaper to harvest and contains more cellulose that can be converted to ethanol. Reconstructed trees should lower the cost of producing and harvesting feedstock from forest plantations, making the tree more attractive for biorefinery operations.

Shorter is better

Research results obtained by Udaya Kalluri suggest that the plant science group at ORNL is on the right path. Kalluri has been focusing on genes known to be associated with elongation of the poplar stem. The genetic blueprint of *Populus* indicates that the tree has 39 auxin response factor (ARF) genes. These unique sequences of DNA bases control the auxin signal response in plants.

Auxin is a major hormone that controls many functions in plants, such as plant development, vertical growth, radial growth, branching and root development, Kalluri explains. Auxin regulates diverse developmental aspects in the plant by conveying the signals from one part of the plant to another.

Kalluri has targeted different ARF genes believed to be responsible for vertical growth. She down-regulated, or decreased the function of, each gene by designing a DNA construct that, when expressed in the plant, causes RNA interference (RNAi). Each expressed gene sends messenger RNA with instructions to the cell's protein-making machinery. In RNA interference certain molecules trigger destruction of RNA from a targeted gene so its encoded protein is never produced.

"We choose an RNAi sequence that has a certain size and DNA base composition specific to the gene we want to disable," Kalluri says. "Then we design RNAi constructs that *Agrobacteria* introduce into poplar tissue. The infected cells that each contain the RNAi construct divide further, producing a callus-like mass of transformed cells.

"We grow the genetically modified plants in our greenhouse," Kalluri adds. "When the saplings are a certain height, we carry out phenotypic evaluation of the genetically modified poplars and determine how their visible features differ from those of poplar trees of the same age."

After three months in the ORNL greenhouse, a wild-type poplar sapling grows to be about three feet tall with a long, slender stem. In dramatic contrast, a genetically modified tree of the same age is only a foot high and has a stocky, leaf-covered stem.

Kalluri and her colleagues showed that genetically modified trees can achieve greater radial growth and less vertical growth than the wild-type poplars. "We have identified some of the genes responsible for the targeted set of traits needed for accelerated domestication of the poplar," she says, adding that the two-year project has been renewed for three more years because of successful results.

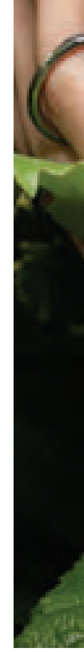
Identifying the right genes

Some hybrid poplars are extremely productive so long as water availability is high. The ORNL strategy is to identify and regulate the expression of the poplar's native gene that makes the tree drought sensitive and increase the activity of genes that enable the tree to pull more water out of the soil.

"We are looking at upregulating, or overexpressing, only genes already present in native poplars," Tschaplinski says. "We will not introduce foreign genes from other species into our plants. Eventually, we will conduct tests to determine which poplar trees designed to be more drought tolerant are as productive as trees without this genetic modification."

Other traits that the ORNL group hopes to incorporate in the genetically modified poplar are cold tolerance, increased ability to take nitrogen from the soil so less fertilizer is needed and branching at the right heights to increase productivity. "Trees tend to grow tall and thin in a crowded environment," he says.

Tschaplinski and collaborators are interested in the chemicals that the poplar makes in response to external stimuli to protect the tree against pathogens and predators. The researchers study poplars grown in plantations at Grand Rapids and Thief River Falls in Minnesota and at Oregon State University in Corvallis. Leaf and root samples from the trees are ground and the plants' chemicals, called metabolites, are extracted. The metabolites are then analyzed.



Poplar saplings in ORNL's greenhouse

A genetically modified poplar is shorter, stockier and richer in leaves (right and left) than the wild-type tree (center).

Using gas chromatography and mass spectrometry, Tschaplinski has identified 58 compounds in the poplar's metabolome, including many carbon-containing phenolic compounds. He is also interested in identifying changes in the chemical content of trees that have been genetically modified for DOE bioenergy and carbon sequestration projects.

As part of a sequestration project, Tschaplinski is creating a genetically modified poplar that makes higher levels of phenolics and other compounds in its roots that are more resistant to breakdown by soil microbes that emit carbon dioxide to the air. "Our hypothesis is that these phenolic compounds are recalcitrant to microbial degradation and, therefore, will stick around in the soil longer," he says.

ORNL is the world's only laboratory involved in identifying, analyzing and modifying poplar genes that code for the production of metabolites of importance to DOE's missions. In addition to the agency's focus on biofuel sources, DOE is also interested in funding studies of how to genetically modify poplar and switchgrass to enhance production in biorefineries of bio-based constituents of commodity chemicals needed to make plastics and nylon substitutes. Of special interest are chemical constituents that are too difficult or expensive to make commercially using petrochemicals.

Should researchers prove successful in making the poplar a solution to America's energy needs, the tree will indeed renew its claim as the "people's tree."—*Carolyn Krause*

Using the System

Learning the function of a single gene or protein is valuable, but science's hopes of great strides in the pursuit of economical bioenergy depend on the ability to understand how components of a living cell or more complex biological systems work together. Such "systems biology" research lies at the heart of the Genomics: Genomes to Life program of the Department of Energy.

Accelerating the domestication and increasing the productivity of poplar trees and other energy crops will require new systems biology approaches. So will improving the efficiency and decreasing the costs of microbial enzymes used to convert wood cellulose to sugar and then ethanol in biorefineries.

At the turn of the century, the possibility of performing systems biology emerged with the completion of various genome sequencing projects, the proliferation of genomic and proteomic data and accompanying advances in experimental and computer simulation methodologies.

Brian Davison, ORNL's chief scientist for systems biology and biotechnology, says that ORNL now possesses the suite of "omics" capabilities that make systems biology possible: genomics, transcriptomics, proteomics, interactomics and metabolomics. "Together these are giving ORNL researchers a deeper picture of how a microbe like hydrogen-producing *Rhodopseudomonas palustris* works, helping identify where improvements can be made by altering protein production coded for by specific genes," Davison says.

In an ORNL project led by Tim Tschaplinski to improve the productivity of drought-stressed poplar trees, researchers used metabolomics to characterize the effects of single gene changes on chemical products of plant metabolism. They analyzed and attempted to identify the genes controlling the production of 58 metabolites made by the normal poplar genome. They also examine the impacts on the plant cell's pool of metabolites of boosting the activity of natural drought tolerance genes to increase water amounts extracted from the soil.

Another ORNL team led by Jonathan Mielenz is applying transcriptomics to understand better the biology of *Clostridium thermocellum*, a bacterium originally genetically engineered at Dartmouth College to improve its unusual ability to convert pure cellulose to alcohol. By studying the bacterium's gene expression using microarrays they developed, they hope to guide modification of the microbe so it can both digest pretreated, impure cellulose from plant biomass and produce pure ethanol fuel.

Early ORNL research results are reinforcing DOE's confidence that systems biology will help researchers break the biological barriers to economical bioenergy.—*C. K.*

The ethanol sector of the U.S. energy market has taken a wild ride from cottage industry to a significant source of renewable fuels for automobiles. Because today's ethanol is produced mostly by fermentation of cornstarch, the emergence of more than 100 American ethanol distilleries is viewed by many as a success story for U.S. agriculture. Despite this expansion of corn-fed ethanol production, some advocates of a long-term solution to alternative fuel needs take a more somber perspective. A valuable source of human food and animal feed, corn ultimately cannot be grown in large enough quantities to supply America's ethanol needs. Moreover, considerable doubt exists as to whether corn-based ethanol represents the most cost-efficient bioenergy solution. Partly as a result of these questions, the U.S. government is showing increasing interest in an alternative to corn. The new plan calls for developing a sustainable industry that would produce ethanol fuel and biologically based chemicals from cellulose-containing trees and grasses using highly efficient, second-generation, fermentation facilities.

Benefits of biofuels

In the Department of Energy's vision, these biofuels and bio-based co-products would be produced in regional "biorefineries" to replace petroleum-derived gasoline for cars and petrochemicals used to make consumer products. Ideally, such a strategy would allay American concerns about soaring gasoline prices, the long-term availability of foreign oil, air pollution and climate change while creating jobs in rural communities and improving the U.S. balance of trade.

Today 4.8 billion gallons of ethanol—about 3 percent of the American fuel supply for cars—are used annually to make E-85 and E-10, reformulated blends of ethanol and gasoline. A clean-burning renewable fuel, ethanol helps gasoline burn more completely, significantly reducing tailpipe emissions that threaten human health and the environment.

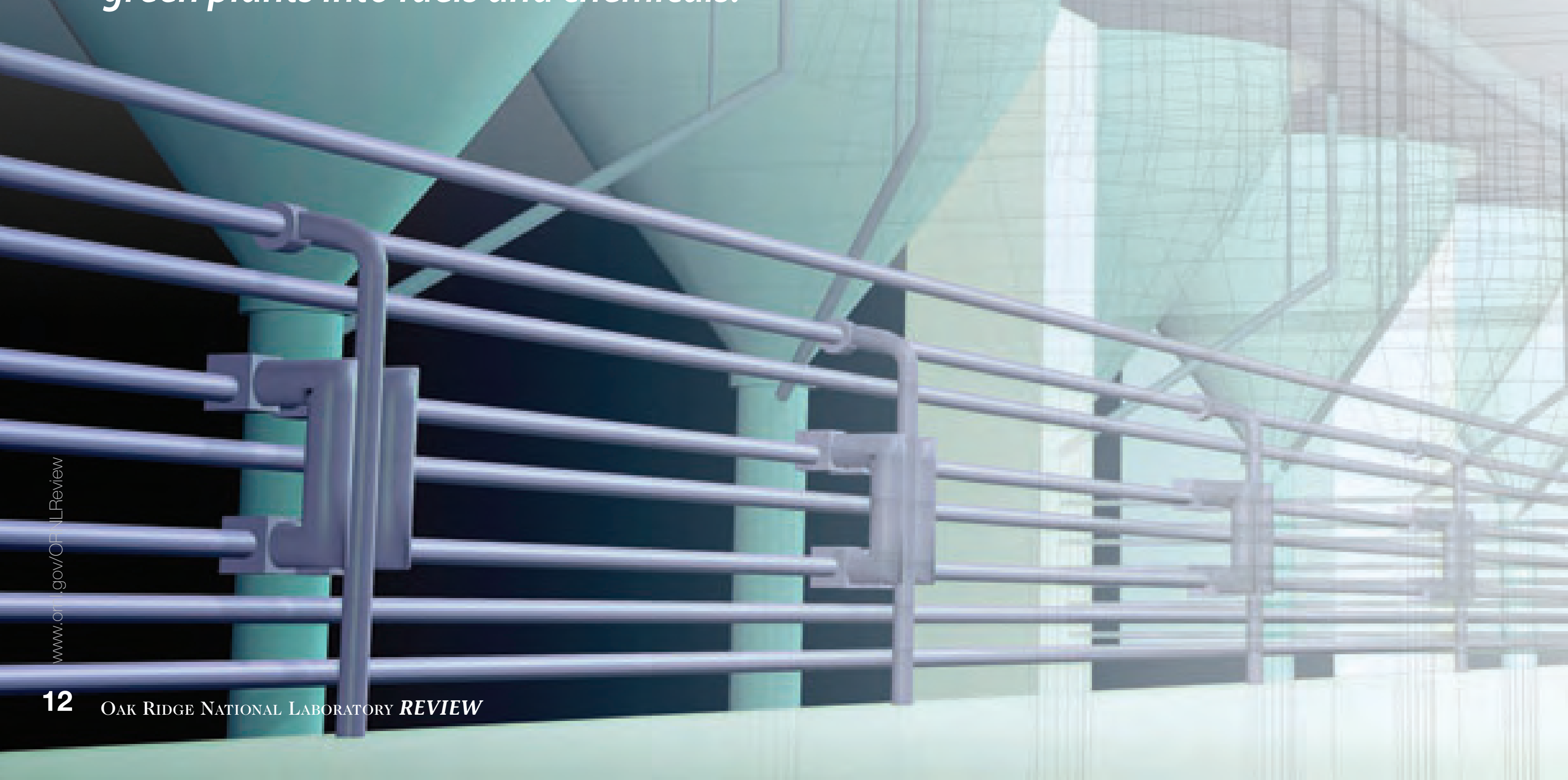
Unlike gasoline, ethanol can be produced from rapidly growing "bioenergy crops" that store carbon absorbed from the atmosphere. Burning a gallon of ethanol barely boosts the total atmospheric carbon that threatens climate change. The reason: the carbon dioxide emitted is almost equal to the amount captured by cellulosic crops used to generate the next gallon.

Studies show that almost one-third more energy is created than consumed by ethanol production, including the energy required for all manufacturing, distribution and agricultural "tractor passes"—planting, fertilizing, and harvesting the corn used as the raw material, or feedstock.

The United States now imports 60 percent of the petroleum Americans use. A government goal is to produce 60 billion gallons of ethanol by 2030 to displace 30 percent of the gasoline needed for personal transportation. "Meeting this goal would

NEXT-GENERATION FERMENTATION

Research aims at cutting costs of turning green plants into fuels and chemicals.



require about 500 biorefineries that each produces 120 million gallons," says Jonathan Mielenz, leader of bioconversion research in ORNL's Biosciences Division. "Corn will certainly be part of the mix, but success will also require cellulosic energy crops. The National Corn Growers Association estimates that 17 billion gallons of ethanol could be produced from corn. The remaining two-thirds of the ethanol will likely come from biomass such as switchgrass and wood chips from harvested hybrid poplar trees."

Ethanol produced from cellulosic biomass would cost about $2.26 per gallon if available on the market today. Another government initiative aims to develop a profitable biorefinery industry—based on new technologies, cellulosic energy crops and value-added co-products—that seeks to lower that cost to $1.07 a gallon by 2012.

In DOE's vision, a biorefinery is a facility that integrates biomass conversion processes to produce fuels, power and chemicals from biomass. The concept is similar to petroleum refineries, which produce multiple fuels—gasoline, jet fuel, diesel fuel and heating oil—and also provide oil to chemical companies that produce petrochemicals for consumer and industrial products. Industrial biorefineries have been identified as the most promising route to the creation of a domestic bio-based industry.

Such biorefineries' profit potential centers on their ability to make affordable ethanol and chemicals from feedstock; produce other chemicals, process heat and electrical power from lignin wastes; and reduce pollution. Maximizing the value in biomass feedstock should enable a biorefinery to produce not only biofuel but also at least one low-volume, high-value "specialty" chemical or one low-value, high-volume "bulk" chemical. The high-value products boost profitability, and the high-volume fuel helps meet national energy needs while lowering fuel costs and reducing oil imports. Added benefits would be the production of power for the biorefinery itself and for the electrical grid, thus lowering energy costs, as well as the avoidance of greenhouse gas emissions.

ORNL's corn connection

Tennesseans have long been familiar with corn, from the hills where illegal moonshine was once produced, to Oak Ridge National Laboratory, one of the nation's leading centers of government-supported, scientific expertise in ethanol production.

Brian Davison, chief scientist for systems biology and biotechnology at ORNL, has helped lay the groundwork for such research through considerable experience producing chemicals from corn. Working with bioreactors, 10-ft.-tall cylindrical columns containing liquids and beads laden with bacteria, Davison and his colleagues demonstrated the production of ethanol, acetic acid, butanol and succinic acid from corn and other feedstock.

Pretreated cellulose from wood chips is broken down by microbial enzymes into sugar, which is converted by microbes into ethanol.

In the 1990s Davison's group and researchers from three other DOE national laboratories demonstrated an award-winning biological method for converting corn to succinic acid at very high yields. Succinic acid is a biologically based chemical that can replace petrochemicals for use in plastics, clothing, paints, inks, food additives and automobile bumpers.

In 1996 ORNL and the three labs signed a $7 million agreement with Applied CarboChemicals, Inc., a Pennsylvania specialty chemical company. The process was licensed to the company, which along with the four national laboratories received an R&D 100 Award from *R&D* magazine in 1997 for being one of the year's top technologies. In 2003 Diversified Natural Products in Scottville, Tenn., was formed from the merger of Applied CarboChemicals and two other companies. DNP will partner with Agro Industrie Recherches et Développments of Pomacle, France, to build a production plant in France. "The French fermentation facility," Davison says, "will produce 'green' succinic acid, which has enormous global demand for everything from industrial solvents and biodegradable polymers to airport runway de-icers."

ORNL also stands to benefit from the neighboring Tate & Lyle facility. Headquartered in England, the company operates the state's only corn-fed ethanol distillery in conjunction with a high fructose corn syrup plant. Tate & Lyle is opening nearby a new $100 million plant in Loudon, Tenn., with partner DuPont that will produce 1,3 propanediol, or PDO, through use of the companies' jointly developed industrial microorganism that ferments glucose extremely efficiently from cornstarch. Bio-PDO™ is a fiber and key ingredient in the production of DuPont™ Sorona®, the newest DuPont polymer that could replace petroleum-derived nylon for uses such as clothing, carpeting and plastics. At least 30 percent less energy is required to produce Bio-PDO than petroleum-based PDO. The company has stated that annual production of 100 million pounds of Bio-PDO will free up enough oil to produce 10 million gallons of gasoline.

Profitable Products

Carpets, drapes, detergents and beverage bottles. Aspirin, vitamins, tires and automobile bumpers. These consumer products, along with athletic footgear, cosmetics, paints, inks, compact discs and cell-phone casings, start with the same raw material: petroleum.

Researchers are convinced that chemical co-products made by reacting catalysts and enzymes with cellulose and lignin from biomass might replace petrochemicals used for consumer products. The result would be more oil available for producing transportation fuel.

The National Research Council estimates that most of the petrochemicals Americans use could be displaced by renewable chemicals from biorefineries and that renewable chemicals could replace about 3 to 4 percent of the petroleum America uses by 2025. Sharon Robinson, manager of ORNL's Industrial Technologies Program, believes that the production of renewable chemicals could help the struggling U.S. chemical industry, which since 2002 has imported more chemicals than it exports, largely because of rapidly rising prices of natural gas used as a chemical feedstock and for process heat.

The primary driver for generating both ethanol and marketable chemical co-products is to make the biorefinery industry profitable and self-sustaining. Biorefineries will churn out most of their renewable chemicals by fermentation of sugars extracted from cellulose and hemicellulose. Pure cornstarch will always have a market because the feedstock is necessary for making impurity-free products, such as polymer intermediates and pharmaceuticals. A Tate & Lyle plant in nearby Loudon, Tenn., ferments cornstarch-derived glucose to 1,3-propanediol, a bio-based replacement for petroleum-derived nylon.

If bio-based chemical feedstocks are produced to replace petrochemical co-products, one concern is that the pioneer biorefineries will swamp the market for many petrochemical replacements. To address this concern, biorefineries should plan to produce co-products with other uses in large volumes. One approach would be for researchers to find ways to capture nitrogen from cellulosic feedstocks to make ammonia fertilizers and animal feed, which could have

Reinhold Mann, ORNL's associate laboratory director for Biological and Environmental Sciences, says that Tate & Lyle is interested in the outcomes of ORNL's bioenergy research and might collaborate with the Laboratory in the future.

Multi-talented microbe

ORNL and its partners are focusing on new methods and technologies for economically converting poplar tree and switchgrass feedstock into fuels. Besides reducing the cost of producing and harvesting the feedstock, the collaborative effort also strives to improve the efficiency of breaking down the feedstock's cellulose and fermenting the resultant sugars.

The plant-based feedstock consists of cellulose (31-49 percent), hemicellulose (16-26 percent) and lignin (19-26 percent). Cellulose in plant cell walls—the most abundant biological material and source of sugar on earth—consists of linked chains of thousands of glucose molecules. This glucose polymer present in corn and cellulosic trees and grasses is the material that is broken down by microbial enzymes into sugars, which are then fermented into ethanol in distilleries and biorefineries.

Cellulose contains six-carbon sugars—glucose. Hemicellulose, a gummy mixture of polysaccharides, contains five-carbon sugars—xylose. Lignin, which makes the plant rigid and resistant to compression, must be removed by a pretreatment consisting of heat, acids and enzymes to make the cellulose accessible to enzymatic breakdown, or hydrolysis, to produce sugar. Microbes, such as yeast, produce enzymes that ferment the sugars to ethanol, which is then separated from the microbes and water by distillation.

The biorefinery's three main processes are pretreatment, cellulose hydrolysis and fermentation of sugar to ethanol and carbon dioxide. To make the biorefinery profitable, researchers are seeking efficiencies in each of the processes. One way to cut costs is to reduce the amount of microbial enzymes needed by genetically maximizing the efficiency of microorganisms known to be effective performers of pretreatment, cellulose hydrolysis and fermentation to ethanol.

One microbe of interest can carry out two of the three processes. Mielenz and other ORNL researchers are examining this versatile bacterium in collaboration with Lee Lynd, a professor at Dartmouth College with whom Mielenz worked, both at the school and in a company the two started. For at least 15 years Lynd has been studying *Clostridium thermocellum*, which can both degrade pure cellulose to make sugar and ferment the sugar to produce ethanol.

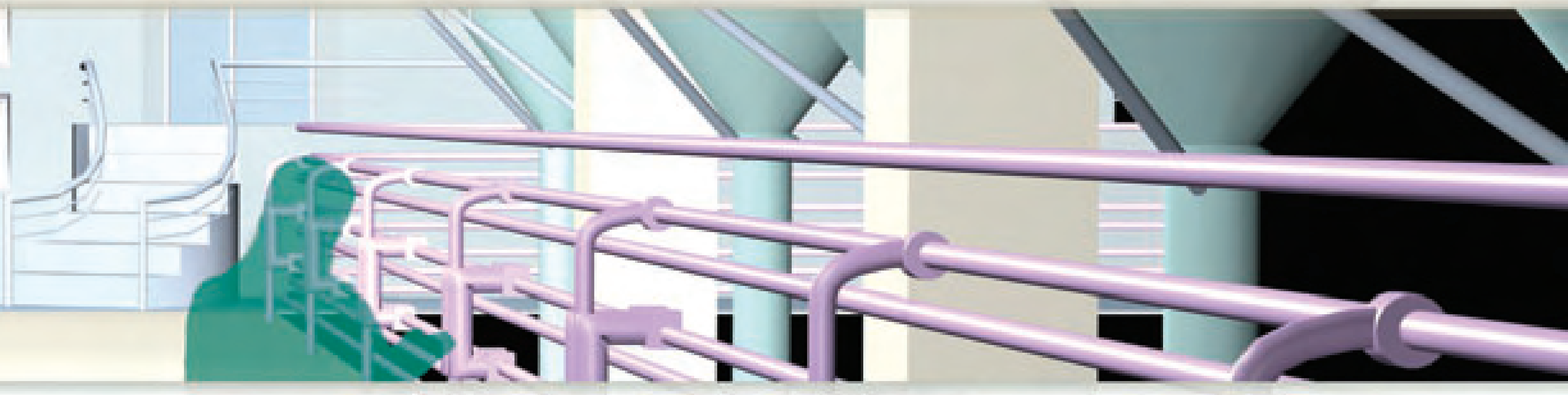
"We have studied how this multitalented microbe makes its own set of cellulase enzymes, grabs hold of cellulose, tears it up, large markets and support numerous biorefineries. Switchgrass, which is 10 percent protein, is a source of nitrogen.

Some biorefineries will burn half their lignin to produce low-value process heat and "biopower" that can be used or sold to the electric grid. An ORNL team hopes to demonstrate that more valuable renewable chemicals can be produced from waste lignin. They have received internal funding to test chemical and enzymatic processes on biomass lignin purified by a technique devised at ORNL.

The researchers predict that because of lignin cleaning and advanced analytical techniques, they can demonstrate that, by using catalysts and biocatalysts to cut ether linkages, they can generate from lignin several aromatic-based compounds similar to petrochemical feedstocks used to make plastics and other high-value products. The group seeks to convince the industry that lignin can be converted into high-value chemical feedstocks as part of a biorefinery operation.

As a result of research funded by the departments of Energy and Agriculture, carbon fiber composites have been found to be one-fifth the weight of steel but just as strong and stiff. If they can be produced more cheaply, carbon fiber composites might replace more steel in cars, making the vehicles lighter and able to use smaller engines and less fuel. Current commercial-grade carbon fiber produced with petrochemicals costs $8 to $15 per pound—too expensive for the automotive industry. ORNL and its partners are developing technologies with an ambitious goal of making carbon fiber for under $5 a pound, a price that could lead to dramatic reductions in the cost of producing lightweight vehicles and in the amount of fuel that new cars consume.

In one of these technologies, new precursors are being developed that could be used to manufacture carbon fibers suitable for automotive composites. The precursors are made by melt-spinning a blend of purified pulp-mill lignin, a co-product of the papermaking process, and recycled plastic. Initial research suggests that lignin from biorefineries could be a similar feedstock for production of carbon fiber composites for vehicles. If the predictions prove accurate, two products from biorefineries—ethanol for automotive fuel and lignin for carbon fiber for automobile bodies—could provide a double benefit to America's environment and energy security by simultaneously reducing greenhouse gas emissions and the nation's need for imported oil.—*C. K.*



accesses the glucose and ferments it to ethanol," Mielenz says. "Part of the biology of *Clostridium thermocellum* is the generation of its own cellulose-degrading enzymes, reducing the fermentation cost because these enzymes do not have to be introduced separately along with added yeast. The bacterium makes more than 20 different cellulases and hemicellulases and other enzymes outside its cell."

Two challenges remain. Biologists do not yet understand how well the microbe will break down pretreated biomass, which is impure cellulose. The microbe also produces impure ethanol—alcohol contaminated with acetic acid and lactic acid. Lynd has led an effort to identify and knock out the genes in *Clostridium thermocellum* that produce the acids. ORNL researchers have produced whole-genome microarrays of *Clostridium thermocellum*, allowing them to identify which of the microbe's genes are turned on during fermentation, actively sending instructions via messenger RNA to the bacterial cell to produce encoded proteins that are enzymes.

"Eventually, we will understand how *Clostridium thermocellum* responds when genes are knocked out in an effort to make the microbe produce pure ethanol free of acetic acid and lactic acid," Mielenz says. "We will also study the gene expression that results when genes are modified in the hope of making the bacterium efficiently digest pretreated, less pure cellulose."

From field to fermenter

ORNL has made contributions to the economics of the bioenergy process because of one group's ability to analyze resource data to determine the locations of the nation's ethanol feedstocks and the costs of bioconversion. Bob Perlack, a resource economist in ORNL's Environmental Sciences Division and lead author of the "Billion Ton" study (see pp. 6–7), continues to analyze biomass feedstock resources considered to be in the supply chain from the field to the fermenter.

An ORNL agricultural engineer, Shahab Sokhansanj, has developed the Integrated Biomass Supply Analysis and Logistics (IBSAL) model. Using Perlack's data, this powerful dynamic model simulates collection, storage and transport operations by optimizing a supply chain for just-in-time delivery of feedstocks to a biorefinery at the least possible cost while meeting quality and sustainability specifications. Recent advances in computational tools have enabled the construction of mathematical models that ORNL researchers are using to simulate supply and transportation of agricultural biomass.

From optimizing microbial fermenters of ethanol to developing models on feeding the process, ORNL and its bioenergy partners are helping lay the groundwork for an economically sustainable biorefinery industry.—*C. K.*

THE BUSINESS OF BIOMASS

Solving the science is only part of the challenge.

Al Womac spends a lot of time chopping switchgrass. The stuff sits in bags, boxes and bales scattered throughout his garage-style laboratory. The lab boasts an array of dicing, mashing, pounding machines—a hammermill, a diskmill, a knifemill and the up-and-coming knife grid that slices up plant matter with the help of a hydraulic ram—along with measuring tools, sifting tools and a conveyor. A researcher at the University of Tennessee, Womac and his colleagues, both from UT and Oak Ridge National Laboratory, are seeking the most energy-efficient means to prepare biomass for conversion into ethanol in a form most conducive to bioprocessing.

As one segment of researchers examines the molecular and genetic questions surrounding bioenergy production, others like Womac are working to resolve issues of how to build a new agri-based industry from scratch. Although more than two decades of research at ORNL and other institutions have laid the foundation for a new bioenergy industry, many "ifs" remain, from growing the crops to transporting and storing the harvested plant matter to preparation of the feedstock for processing.

No existing commercial plants yet make ethanol from lignocellulosic feedstocks—the tough, fibrous content of plant stalks, leaves and stems. The cost is still prohibitive, approximately $2.26 per gallon versus $2.11 for corn-based ethanol, according to the latest government figures. Part of the cost conundrum can be answered by science. "But then by the same token I realistically have to be able to grow, transport and store feedstocks economically, environmentally and sustainably," says Mark Downing, agricultural economist at ORNL.

At UT and ORNL, researchers are paying particular attention to issues surrounding switchgrass, which has been identified as an easy, alternative crop for local farmers. The grass, still currently used as a forage grass crop, was identified in the late 1970s as a potential "model species" for any herbaceous crop. Switchgrass once carpeted large portions of the American prairie where buffalo herds roamed. The hearty plant grows at least eight feet tall in any climatic variation, from the Gulf Coast into Canada.

Despite the apparent ease of growing switchgrass, Downing ticks off a laundry list of concerns: How can a biofeedstock supply be created before cellulose-based ethanol refineries are built? Which are the best switchgrass varieties? How often should a farmer plant and harvest? What are the environmental consequences of a so-called "monoculture crop" that could span vast acreage across the nation? Can a low-value commodity with, essentially, the low-bulk density of toilet paper be transported economically? What is the best method of preparing biomass for processing? How and where would the grass and trees be stored after harvest?

A number of Department of Energy-funded projects involving Oak Ridge National Laboratory and other institutions are examining these and other questions that accompany the creation of a major new industry.

Supply or demand

At Iowa State University, for instance, a project launched more than 15 years ago to market grass crops in the southern part of the state has evolved into research on commercial production of switchgrass. In this case the grass is fed to a nearby power plant, but the production has obvious implications for the bioenergy industry, says Downing, who has been working with the university. Farmers there have planted more than 6,000 acres of switchgrass on both Conservation Reserve Program land and some less productive corn-producing acreage.

Through the years researchers have evaluated a variety of issues, from how best to harvest the grass to the impacts of planting and harvesting on local bird populations. “We’ve got farmers out there in the back shop with welders going to town developing machinery to harvest and manage crops,” Downing says. “Environmental issues are very big. Some environmental advocates are uncomfortable with monoculture production or cutting trees along streambeds, so we are examining which techniques offer farmers the best advantage to the environment as well as economic benefits to farmers. A number of similar tradeoffs affect the economics. We are at a very fledgling stage in understanding how we should manage crops for fuel.”

A key to the growth of the biomass industry is the potential genetic modification of crops such as switchgrass and poplar trees for higher production, drought tolerance and resistance to disease. The research brings with it concern that such genetic modification could affect native communities and prove detrimental to surrounding ecosystems.

“We do not fully understand the effect of genetically modified crops on native populations,” says Neal Stewart, who holds the Racheff Chair of Excellence in UT’s Department of Plant Sciences. Such crops not surprisingly undergo a high degree of government regulation, a hurdle that farmers and biorefineries must overcome.

These issues can be addressed, Stewart is quick to add. “I think bioenergy will create an agricultural revolution,” he says.

Researchers and farmers are still learning the basics of growing crops for bioenergy. In another project, managed by the University of Tennessee, researchers are experimenting with various ways to grow switchgrass using several plant varieties and varying levels of fertilization. The experimental plots are situated on 32 acres at UT’s Research and Education Center at Milan in West Tennessee.

“We chose four distinctly different soil and landscape positions that represent the different soil and area compositions for this part of the state,” says Don Tyler, UT soil management researcher. “On each position we have two experiments, one looking at different seeding rates and one at different nitrogen rates for switchgrass production.” Another experiment compares traditional native switchgrass with three “synthetic” cultivars, bred for improvements in production and early seedling vigor.

Through another UT project, funded by the Department of Energy, the university has set up contracts with five farmers in two Tennessee counties to grow 92 acres of switchgrass. The project aims to uncover the challenges and economic viability of raising the bioenergy crop, says Kelly Tiller, agricultural economist at UT.

“The goal is to make this a competitive option for the farmer,” Tiller says. “One of the nice things about this crop is that switchgrass is a perennial. Once the plant is established, the cost of production is minimal. With switchgrass, farmers do not need to see the same level of market returns as with corn or soybeans because they do not have as much invested in the crop.” In addition, she says, “switchgrass can be grown on much more marginal cropland.”

The project is experimenting with some different types of contracts, including yield-based payment, fixed payment and a combination of the two, allowing farmers to determine which concept works best and to document production on their land.

Farmers have been more than willing to sign up for the program, but launching full-fledged switchgrass production for biofuel production reveals "a classic chicken-and-egg problem," Tiller says. "If farmers grow switchgrass today, there is no market. On the other side, if companies want to build processing plants, they need a supply of switchgrass. One side has to move first—probably the demand side. If the demand is there, I think that agricultural production could ramp up pretty quickly."

Researchers at the University of Tennessee are exploring a variety of ways to chop and otherwise prepare switchgrass and corn stover for potential use as a source of biofuel.

After growing the biomass crops, farmers and bioprocessing companies must then determine how best to transport biomass to the biorefinery as well as how to store the harvest in the meantime. Some farmers are baling switchgrass; others are simply leaving the harvested and chopped switchgrass in piles on the field, where Downing says the grass naturally forms a lattice configuration that protects the crop from the elements. There are also issues related to "the whole process of detwining, de-baling, chopping and blowing the switchgrass as the biomass is fed into a biorefinery," Downing says. "You would think it would be easy but it's not."

Slicing and dicing

That brings us back to Womac—the UT researcher who is, as Downing says, "chopping the daylights out of switchgrass."

Womac's research group, funded through the U.S. Department of Agriculture–DOE Joint Biomass Research and Development Initiative, has practiced a variety of methods in cutting switchgrass and corn stover in search of the perfect combination of maximum surface

Tennessee Steps Up

On Jan. 31, 2007, Gov. Phil Bredesen joined with the Tennessee General Assembly's House and Senate speakers in a commitment of $72.6 million toward what the governor called a "transformational effort" to make Tennessee a model for biology-based energy production.

In what the governor termed a "farm to market" approach, the plan calls for a partnership between the University of Tennessee and Oak Ridge National Laboratory with a long-term goal of producing 1 billion gallons of ethanol from switchgrass, a volume that represents approximately 30 percent of the state's current gasoline consumption.

The plan contains a comprehensive, three-part strategy that includes increasing the production of agricultural commodities, overcoming the scientific and technological challenges to producing cellulosic ethanol at a competitive cost, and construction in Tennessee of the nation's largest pre-commercial demonstration plant for production of ethanol from switchgrass.

Tennessee's investment includes $24.6 million for research activities, research equipment and a new research facility dedicated to bioenergy and located on the campus of Oak Ridge National Laboratory. Research at the University of Tennessee College of Agriculture will focus on increasing the current yield of switchgrass, a crop that can be grown in virtually every region of the state. The plan anticipates the need for a five-year period to subsidize the growth of switchgrass as farmers make the transition from tobacco and other crops.

The plan's most ambitious undertaking is the construction of a demonstration plant capable of producing 5 million gallons annually of ethanol. Owned by the University of Tennessee and managed by a private company, the plant will provide the critical element needed to demonstrate the commercial viability of new processes developed at ORNL for producing ethanol from cellulose in switchgrass and other crops.

The state of Tennessee's investment comes in support of a proposal by an ORNL-led consortium to host one of the Department of Energy's Bioenergy Research Centers. ORNL's proposal seeks to remove biomass recalcitrance—cellulose's natural resistance to being converted to sugar—as a barrier to cost-effective production of biofuels. Should this ambitious goal become a reality, the result could be a dramatic impact on America's consumption of transportation fuels.

Tennessee's investment is among the largest ever made in support of bioenergy. The state is betting on a return that could indeed be transformational.

area—for easiest breakdown of the plant into cellulose—and energy efficiency. To that end, the researchers are collecting measurements using sensors planted inside the various chopping, knifing and clubbing machines to determine variables such as the point at which a plant breaks most easily, the kilowatt hours per ton required to chop the material and the feed rate into the chopping machines.

One project involves running samples through sieves. In another exercise, a graduate student, aided by a computer scanner and software package, counts the fragments of a particular sample in order to classify by size the particles that shoot out the other end of the chopping equipment. The information is necessary to determine ideal particle size for bioprocessing and to address environmental considerations in designing and operating a biorefinery, Womac says. "Fugitive dust emissions create a whole new set of issues," he says.

UT, through collaboration with ORNL, is also working with industry to receive feedback on the research and, eventually, integrate the data into commercial processes. Each step of the way, bioenergy companies and researchers must be guided by whether the energy cost of creating biofuel exceeds the payback. In that context the model for biofuel production appears to be very localized in nature, Downing says. Because ethanol's corrosive properties prevent the fuel from being transported via pipeline, and because the costs of transportation and storage are often prohibitive, ethanol production will likely be housed in facilities that serve local regions within a state, or even a county.

With this in mind, DOE has funded an initiative to "begin assigning a matrix of costs and a projection of expectations for the handling, management and qualitative aspects of crops generated for biofuel" on a region-by-region basis. Known as Regional Feedstock Partnerships, the effort has motivated many government agencies—federal, state and local—to begin the process of planning for a future in which fuel flows not from oil fields but from nearby fields of switchgrass, corn and trees.

"Let me tell you, when we get these challenges worked out, everybody is going to want a piece of the action," Downing says. "The results will open up wonderful opportunities for lots of sectors in the U.S. economy."—*L. B.*

ENZYMES IN MOTION

ORNL's supercomputer shows how microbial enzymes turn plant cellulose into sugar.

Harnessing the capabilities of one of the world's most powerful supercomputers, the largest biological simulation ever conducted at Oak Ridge National Laboratory is providing insights on converting cellulose from green plants into sugar. The supercomputer's ability to create a visualization of a million atoms promises to help researchers design more efficient methods for producing biofuels.

Like humans, microbes depend on sugar for energy. Fungi and bacteria obtain sugar from cellulose, the glucose polymer that composes cell walls in trees and other plants on land and in the ocean. These microorganisms produce cellulases, enzymes that work together to extract glucose from cellulose and turn the sugar into energy.

Computational biologists from ORNL and the National Renewable Energy Laboratory in Colorado, along with a researcher from Cornell University, are modeling bacterial and fungal cellulases in action at ORNL. Researchers "watch" these simulated enzymes attack digital cellulose strands, transfer a strand's sugar molecules to the enzyme's catalytic zone and chemically digest the sugar to provide the microbe with energy. The key to increasing the efficiency and lowering the cost of ethanol production using sugar from cellulose in trees and other biomass is to understand how cellulases degrade cellulose. Such understanding may lead to genetic engineering of the degradation mechanisms, speeding the biofuel production process.

John Brady of Cornell developed the original model of a cellulase molecule processing cellulose fibers under an optical microscope (see image on p. 21). Led by NREL's Mike Himmel, other collaborators include Ed Uberbacher and Phil LoCascio, researchers in ORNL's Genome Analysis and Systems Modeling Group, and Pavan K. Ghattyvenkatakrishna, a University of Tennessee graduate student who works in the GASM Group.

"We are studying the dynamics of cellulase at work on cellulose," says Uberbacher. "The model's cellulose resembles wood under a microscope. The individual strands are sugars strung together as a long polymer chain. The cellulase enzyme comes down and pulls a strand from the bundle forming the glucose polymer. The cellulase feeds the sugar fiber up to another domain of the enzyme that catalyzes the removal of the six-carbon sugar from the fiber. The process is a crucial step in making ethanol fuel from biomass."

The goals of the project include understanding how the cellulase enzyme functions, how it recognizes cellulose strands and how the chemistry is accomplished inside the enzyme. The group also hopes to determine what the rate-limiting steps are that might be genetically engineered to make cellulase more efficient at degrading cellulose into glucose.

The ORNL team performs the modeling using molecular dynamic simulations on 1,000 to 2,000 processors of "Jaguar," the Laboratory's Cray XT3 supercomputer. Jaguar, part of the Department of Energy's National Center for Computational Sciences, will perform more than 100 trillion calculations per second this year. Visualization in the nearby EVEREST lab has sparked new hypotheses and insights into how the enzyme flexes its shape and

Science National Champions

Oak Ridge High School's Scott Molony, Scott Horton and Steven Arcangeli win a $100,000 scholarship for their bioenergy project.

In December 2006 three Oak Ridge boys won the high school equivalent of a Nobel Prize in science and a $100,000 scholarship by collaborating on a bioenergy project with their mentors from ORNL. The Oak Ridge High School team of seniors Scott Molony, Steven Arcangeli and Scott Horton (whose parents Linda and Joe Horton work at ORNL) placed first in the Siemens Competition in Science, Math & Technology, the nation's premier high-school science competition. The contest was held Dec. 1–4 in New York City, and U.S. Secretary of Education Margaret Spellings presented the award. Earlier, the ORHS seniors won a $6,000 scholarship in the Siemens competition by finishing first in their region. Their championship work also netted $2,000 for the school's science program and helped their mentors—computer scientists Nagiza interacts with the solid substrate. Each simulation to test ideas about how the enzyme works runs for a number of days.

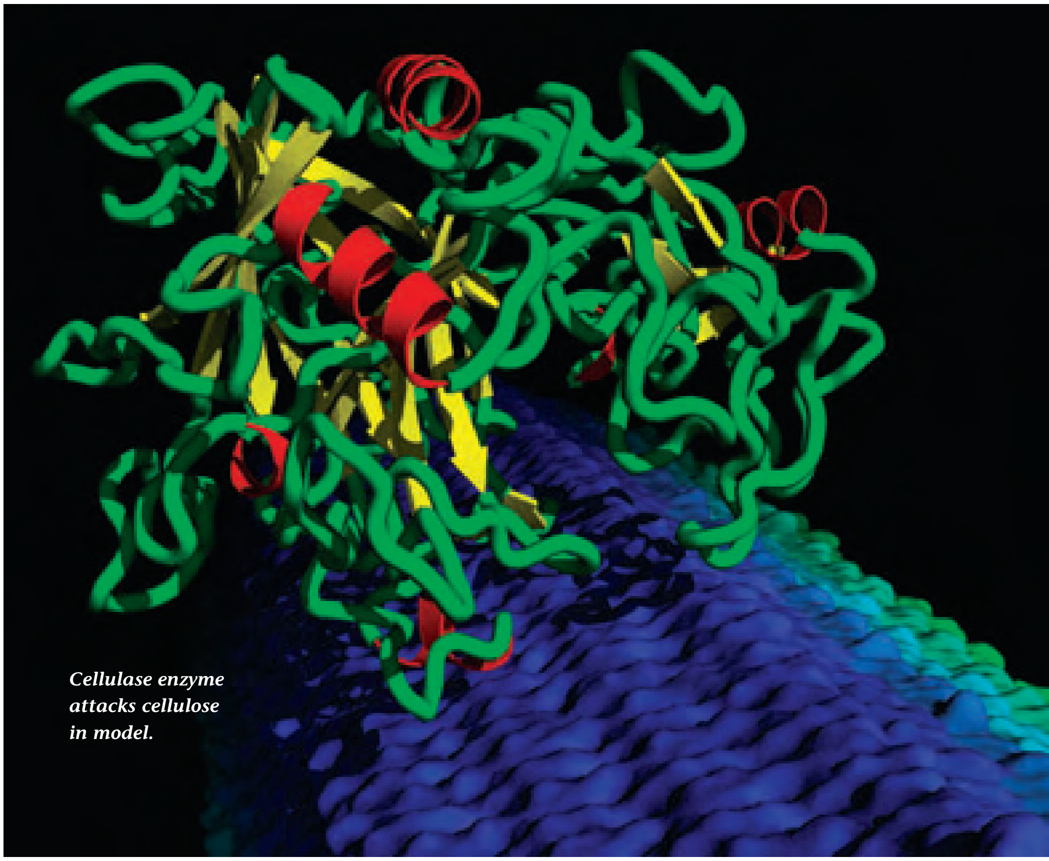
"Cellulase works one 1,000 times slower than most enzymes in our bodies," LoCascio says. "It takes perhaps 100 nanoseconds for this cellulase to move down one cellulose fiber and clip off a sugar molecule."

Jeremy Smith, molecular biophysicist and the first joint Governor's Chair appointee at UT and ORNL, uses both computing and neutron scattering to examine the positions and motions of atoms in cellulose-digesting enzymes. (See interview on pp. 22–23.)

"Humans want to make alcohol out of plants, but plants do not want to be made into alcohol," he says. "We hope to learn why the enzymes we introduce do not degrade cellulose very fast and why plant cell walls will not cooperate and break down quickly."

Smith conducts neutron studies and simulations of cellulosomes, spider-like molecular machines that microbes create outside their cells to degrade cellulose effectively. "While working at the University of Heidelberg in Germany my colleagues and I published work on how cellulosome components talk to each other," he says, adding that he plans to continue his cellulosome research using the backscattering spectrometer at ORNL's Spallation Neutron Source.

Computational biologists hope to explore the diversity among cellulases and figure out why some cellulases work better at extremely high temperatures while others prefer lower temperatures. LoCascio points out that ocean bacteria, which live in extremely hot thermal vents and have no access to sunlight, make cellulases that degrade ocean biomass. One question researchers hope to address is how fungal cellulases that extract sugars from tree cellulose differ from bacterial cellulases produced on the forest and ocean floors under different conditions.—*C. K.*



Cellulase enzyme attacks cellulose in model.

Samatova, Tatiana Karpinets, Hoony Park and Chris Symons—win $800,000 in internal funding from ORNL's Laboratory Directed Research and Development program. Samatova had mentored an ORHS team that placed fourth in the 2005 Siemens competition, making the 2006 win the first time the competition has had repeat finalists from the same school.

Both winning teams came from ORHS calculus teacher Benita Albert's "Math, Science, Computer Science Thesis" class. Last spring when Samatova talked to this class about her research, she suggested that bioenergy, an ORNL strategic research direction, could be a winning Siemens competition topic. Last summer Albert sent six students to ORNL where they learned about the systems biology supercomputer tools developed by Samatova's team and read papers and presented seminars on bioenergy, filling gaps in the researchers' knowledge.

The winning team worked long days June 1 through August 11, 2006, at ORNL learning graph theory, statistics, bioinformatics, systems biology, artificial intelligence and programming in C++. Scott Horton expressed interest in applying ORNL supercomputer tools to biology questions, so for their thesis the three boys chose to evaluate how well these tools could be applied to understanding the mechanisms by which microbes efficiently convert biomass to ethanol. Focusing on 28 bacterial genomes, half of which grow in oxygen and half of which do not, the boys wrote programs to identify genes and biochemical pathways linked to traits that are important to the industrial conversion of biomass to ethanol—resistance to high temperature, metabolism of multiple sugar types and high ethanol yield. They improved ORNL codes to allow two supercomputers to better handle high volumes of data. Last autumn, they continued their research an hour a day in their "math thesis" class and every Wednesday afternoon at ORNL.

Applying their graph-theory methodology to *Zymonas mobilis*, an industrially accepted bacterium for bioethanol production, the boys found their computational results agreed with experimental results on the same microorganism published in a *Nature Biotechnology* paper. The students' methodology, when applied to thousands of microbes, might suggest ways to genetically endow a microorganism with a collection of traits needed to engineer an incredibly high yield of ethanol—and maybe dollars.—*C. K.*

JEREMY SMITH

In 1991 he published a 64-page review article on neutron scattering in biology. The last sentence referred to plans, then on the drawing board at Oak Ridge National Laboratory, for a new reactor-based neutron source called the Advanced Neutron Source, concluding: "We await their fruition with some excitement."

Ultimately, plans for the ANS were dropped and subsequently replaced by the accelerator-based Spallation Neutron Source, whose first neutrons flew last spring. Meanwhile, Smith was developing his résumé as an internationally renowned molecular biophysicist with a penchant for combining neutron scattering with high-performance computer simulation to understand the physics of biological molecules. Smith built two successful interdisciplinary groups, first at the French national laboratory at Saclay, near Paris, and then at the University of Heidelberg. Having turned down offers of professorships in six countries, last fall Smith became the first University of Tennessee-Oak Ridge National Laboratory Governor's Chair and Director of the ORNL Center for Molecular Biophysics.

Smith says he was attracted to Oak Ridge both by the SNS and by the establishment of the Laboratory's Leadership Computing Facility, which will this year become home to one of the fastest open-science supercomputers in the world.

Briefly describe your research background.

I decided to leave Britain at the age of 22. The choice was then either to go to graduate school at Yale or to work in the south of France, at the Institut Laue-Langevin in Grenoble, which at the time had the world's best neutron source. The Ph.D. work in France was quicker, the pay better, and I also liked the idea of learning a foreign language and how to ski. And I was really keen on French women! So Grenoble is where I started research into probing motions in proteins with neutrons, and I have been involved in this field for the last 25 years. The results of the neutron experiments in Grenoble needed interpreting, which I learned to do with computer simulation. We initiated a research field that combines these two techniques and is now clipping along nicely. I subsequently spent four wonderful years learning computational chemistry at Harvard and then tried to reproduce the creative atmosphere there in my own two research groups, in Saclay and Heidelberg.

What are some specific ways you'll be able to apply the Spallation Neutron Source and Leadership Computing Facility to your research?

With a neutron source, like the SNS, which instruments you build determines what kind of science you can actually do. SNS has decided to build instruments that will aid in the study of materials. That is perfect for biology, because biology is, in a way, just the study of particularly beautiful and complex materials. So many of the planned instruments will be useful to us. To interpret the experiments we will need to do large-scale simulations using the Laboratory's supercomputers, from which we will calculate the neutron scattering spectra and understand them. High-performance computing will also be useful for understanding a range of other problems not directly accessible with neutrons.

How will your research aid in bioenergy production?

I'm involved in research related to hydrogen production and bioethanol. We hope to understand how hydrogenase enzymes work. These are very clever enzymes that enable bacteria to evolve hydrogen and use it as a metabolic agent. You just take one mole of this enzyme and in only two hours you can produce enough molecular hydrogen to fill the main liquid hydrogen tank of the space shuttle. We need to understand how hydrogenases work and then build robust synthetic nanoscale mimics. For bioethanol production, if one can chew up plant cell-wall cellulose into sugars then one can make ethanol out of the sugars pretty easily. The problem is plant cell walls are recalcitrant to being chewed up. So we would like to understand what about cell walls makes them recalcitrant, by combining computer simulation and neutrons again. Now microbes produce special molecular machines that do overcome cell-wall recalcitrance and we want to find out how they work, too. Once you've understood these processes, you can think about doing them yourself.

What other areas of research are you involved in?

We've been involved in designing an instrument based on single-molecule spectroscopy that detects many cancers very early and works very well. We are also involved in AIDS research, designing vaccines using computer simulation. Another longstanding interest of ours is another field of research that the Department of Energy is potentially interested in, the atomic-detail physics of photosynthesis—biological light-driven energy transformation. For example, one particularly interesting purple protein absorbs light and then uses the energy to pump protons across a membrane. We are very interested in finding out how that works, and the principles we learn could also be useful in fuel cell design. More generally we want to understand enzyme reactions and how enzymes use chemical energy to make molecular machines work, such as the proteins in muscle contraction, vision or cancer-cell growth. We are also trying to find out why cholesterol was chosen by nature to be incorporated into biological membranes, rather than some other similar molecules that are easier to make.

Will you teach classes at the University of Tennessee?

Yes, certainly. Molecular biophysics sits exactly at the junction of biology, physics, chemistry and computer science, and so here at ORNL I find myself positioned among four directorates—those of biological and environmental sciences, computational sciences, physical sciences and neutron sciences. And I have much in common with all of them. Likewise, for teaching we require students with strong interests in physics and chemistry, who are also OK with math and computers, but are driven by a desire to understand biological systems. What I'd like to do is set up an international, elite UT-ORNL graduate program in molecular biophysics that I would teach with the ORNL research staff and UT junior faculty who will be associated with my Governor's Chair. I am sure we could attract top students from various backgrounds who have the mental agility for strongly interdisciplinary study. I think an important part of my work will be to help stimulate interaction between UT and ORNL. Both have a lot to win from forging stronger links. Oak Ridge needs more hyperactive, caffeine-drinking, midnight-oil-burning graduate students to get the research done, and UT needs to make optimal use of the facilities here in order to elbow up in the university research rankings. Both badly need this synergy.

You are an avid soccer fan and a skilled player. What is your take on American football?

I'll tell you one thing: no European has any idea what college football is about. I'll lay a quid that if you went to any Frenchman in a Grenoble brasserie and asked, "What if I were to float the idea to you of 104,000 people crowding into a stadium in East Tennessee seven times a year, all wearing strident orange and fervently identifying with a bunch of inexperienced college students running around wearing motorcycle helmets?" he would retort, "Are you kidding me? No way!"

TAKING THE LONG VIEW

Hydrogen produced using algae, water and sunlight could be a long-term energy source.

While some ORNL researchers strive to develop a cost-effective means of converting green plants to ethanol and other liquid transportation fuels, their colleagues are exploring another potential plant-based source of renewable fuel for the longer-term goal of hydrogen-powered vehicles.

The development of hydrogen as a major energy carrier envisioned for the latter half of this century includes the use of green plants to produce hydrogen to power fuel cells in electric cars, replacing internal combustion engines and dramatically slowing the buildup of atmospheric carbon dioxide. The Department of Energy views the use of hydrogen as one way to address the agency's energy security and environmental missions.

"Green" hydrogen sources

After America's first major energy crisis in 1973, some researchers at the national laboratories began exploring photosynthesis to extract hydrogen from water in the search for energy alternatives. Three decades later, two common methods for producing hydrogen use fossil fuels and release carbon dioxide, a greenhouse gas. In one method, hydrogen is produced by reacting natural gas with steam at high temperature. Splitting water molecules using electrolysis—which often uses electricity from power plants that burn coal, natural gas or oil—also produces hydrogen.

ORNL was the first research institution to demonstrate the sustained simultaneous production of hydrogen and oxygen by illumination of green algae, a biological version of electrolysis, for hydrogen production. However, the efficiencies of the process must be improved before the research will have practical application.

The research was pioneered by Eli Greenbaum, an ORNL corporate fellow who heads the group in the Chemical Sciences Division that demonstrated a way to split water into hydrogen and oxygen using algae in the presence of light. The team is currently using genetic engineering to make a mutant form of algae with the goal of boosting photobiological hydrogen production 10 times using light with a tenfold increase in intensity.

In 1999, 60 years after a scientist observed that pond scum algae alternated between hydrogen production and normal photosynthesis in different atmospheres, researchers at the University of California at Berkeley and DOE's National Renewable Energy Laboratory in Colorado determined that depriving algae of sulfur and oxygen enables the production of hydrogen for an extended period. Plants require sulfur to survive because they make proteins from the element. Eventually, researchers were able to switch hydrogen production on and off repeatedly by changing the algae's chemical environment.

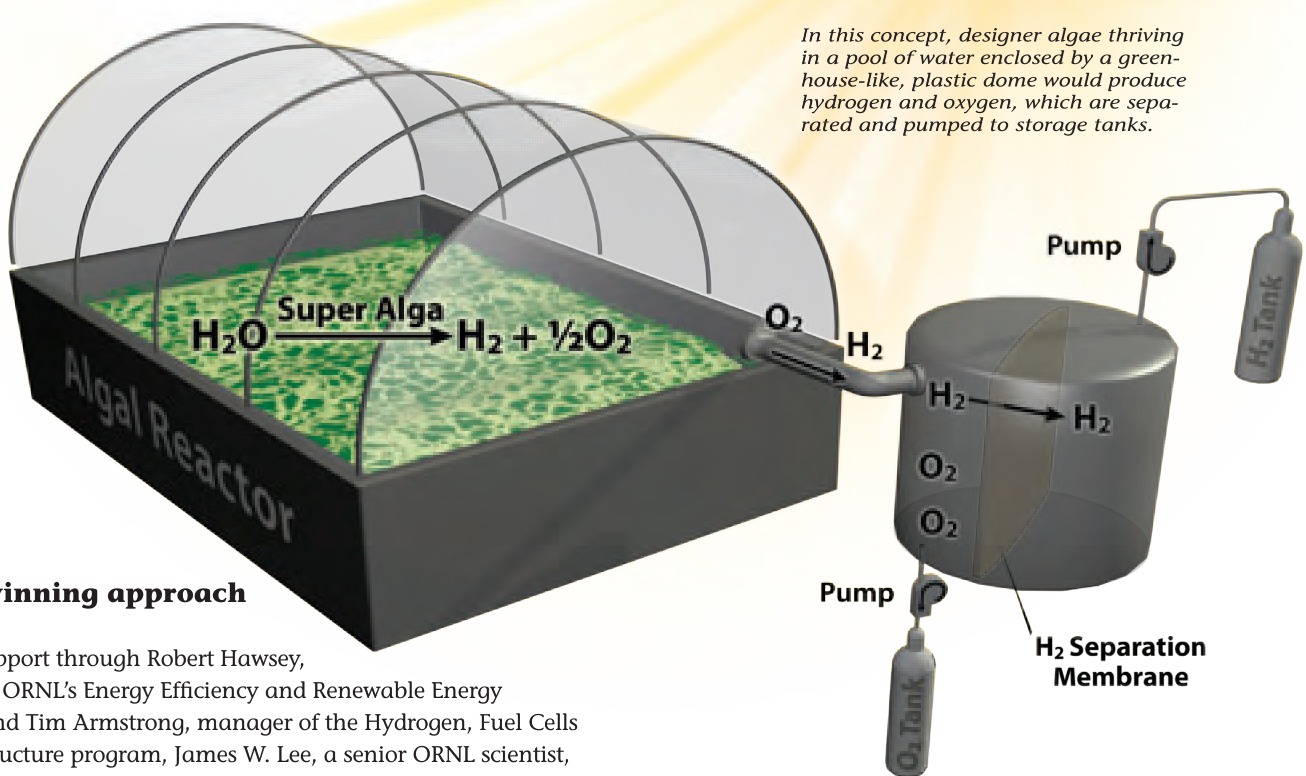
In Oak Ridge, Greenbaum's group discovered that *Chlamydomonas reinhardtii* can produce sustained simultaneous production of hydrogen and oxygen from water using light for extended periods of time. These algae normally grow new cells by photosynthesis, using carbon dioxide from the air in the presence of sunlight. But after placing the aquatic organisms in a large flask of water illuminated by lamps, the ORNL researchers "tricked" the algae by depriving them of carbon dioxide and oxygen. As a result, a normally dormant gene becomes activated, leading to the synthesis of the enzyme hydrogenase. The algae use this enzyme to produce both hydrogen and oxygen from water.

"Our group performed some of the original basic research studies on the kinetic rates and mechanism of photosynthetic hydrogen production in which green algae split water into molecular hydrogen and oxygen," Greenbaum says. "We were the first to demonstrate that illuminated green algae can be used to sustain the simultaneous production of hydrogen and oxygen. We performed the first measurements of the photosynthetic unit size and turnover times of hydrogen and oxygen production."

Greenbaum made another important discovery. His research also demonstrated that the presence of carbon dioxide inhibited photosynthetic hydrogen production.

A Chevrolet Equinox hydrogen-powered, fuel-cell vehicle.
General Motors photo by Steve Fecht

In this concept, designer algae thriving in a pool of water enclosed by a greenhouse-like, plastic dome would produce hydrogen and oxygen, which are separated and pumped to storage tanks.



Award-winning approach

With support through Robert Hawsey, manager of ORNL's Energy Efficiency and Renewable Energy program, and Tim Armstrong, manager of the Hydrogen, Fuel Cells and Infrastructure program, James W. Lee, a senior ORNL scientist, leads the ORNL photobiological hydrogen research effort using a new approach: proton-channel designer algae for enhanced hydrogen production from water. Lee developed this new approach using molecular genetics based on the fundamental understanding of biological hydrogen systems that has accumulated in the field, including Greenbaum's pioneering contributions.

The proton-channel designer alga approach could solve the following four problems that currently challenge researchers and investors in the field: (1) restriction of photosynthetic electron transport needed for hydrogen production by the increased proton concentration gradient, (2) competitive inhibition of photosynthetic hydrogen production by carbon dioxide, (3) requirement of bicarbonate binding at photosystem II (PSII)—a protein in the algal chloroplasts which absorbs light energy—for efficient photosynthetic activity, and (4) competitive drainage of electrons by oxygen in algal hydrogen production. Lee says that, unless these four physiological barriers are overcome, impressive amounts of hydrogen will not be produced from green algae.

"For example, the biomolecular machinery needed for hydrogen production severely stalls when the algal thylakoid membrane is quickly jammed with too many protons, inhibiting photosynthetic electron transport," Lee explains. "In addition, natural algae do not produce hydrogen efficiently because of the competitive inhibitions by carbon dioxide and oxygen. Furthermore, because the binding of bicarbonate at PSII is required for efficient photosynthetic activity, the inhibition of hydrogen production by the presence of carbon dioxide cannot be solved by removal of this source of carbon."

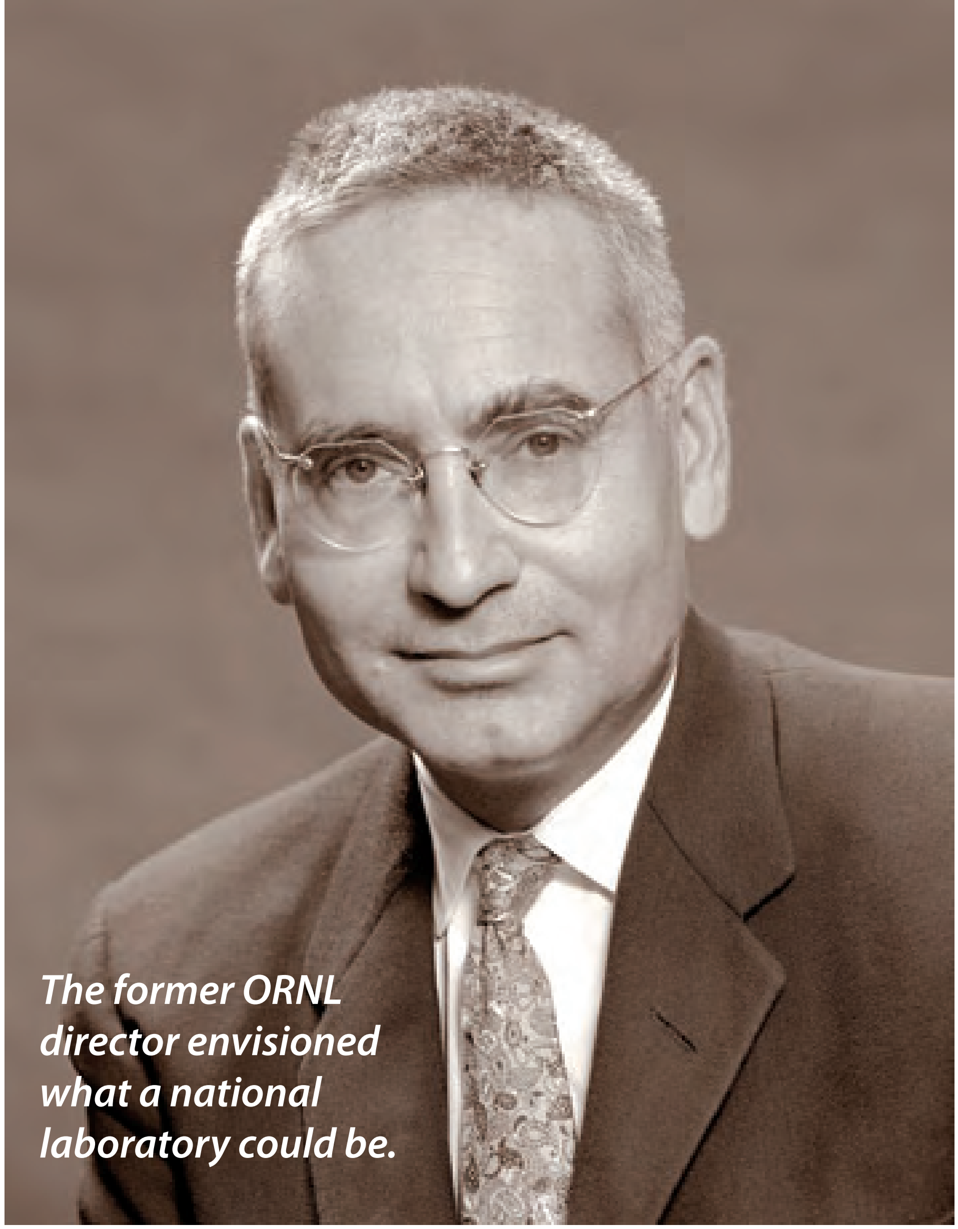
However, according to Lee, these four problems could be simultaneously solved by the proton-channel designer alga approach. The reason: all four hurdles are associated with the proton concentration gradient.

In supporting Lee's project of genetically engineering wild algae to leap over all four hurdles, Dong Xu used the award-winning PROSPECT computer software tool he helped develop at ORNL to analyze the structure of mellitin, or bee venom, which conducts protons. With this model, Lee and his collaborators designed a proton-channel gene and coupled it with another DNA segment that serves as a promoter, turning on only when oxygen is absent. Thus, the proton-channel gene is expressed only when not exposed to oxygen. During those times, protons pass through the channel the gene creates, preventing proton accumulation and simultaneously eliminating the other three proton-associated problems as well.

"We have made our first set of proton-channel genes and introduced them into algae cells successfully," Lee says. "We could improve renewable production of hydrogen from water by a factor of more than 10 if the designer alga gene works as theory indicates. When we remove oxygen, the designer gene should switch on, causing the mutant algae to produce hydrogen in large amounts."

Lee, who received the FuelCellSouth 2006 Crystal Flame Innovation Award for this research, is realistic about the challenges that remain: "In addition to creating the designer algae, we will also have to solve engineering problems, such as separating hydrogen from oxygen and suppressing the explosive potential of hydrogen in the presence of oxygen," Lee says. "Our 'switchable PSII designer alga' concept, which has recently been explored through our ORNL seed money project, could provide an alternative solution to the problems posed by the presence of oxygen, including the need to separate oxygen from hydrogen immediately after both gases have been produced from biological splitting of water molecules. Calculations indicate that the designer algae hydrogen production technology, when fully developed, could annually support 140 fuel-cell cars per acre of enclosed algal ponds. This estimate represents a theoretical upper limit, and much more work is needed to achieve such a challenging goal."—C. K.

Alvin Weinberg (1915–2006)



The former ORNL director envisioned what a national laboratory could be.

Alvin M. Weinberg in many ways personified Oak Ridge National Laboratory. As the Laboratory's visionary director and the intellectual leader of an energy policy think tank he founded at Oak Ridge Associated Universities, he influenced U.S. government energy and science policy as well as research funding priorities—from reactor design and nuclear safety to renewable energy and the impact on climate of increased carbon dioxide emissions from coal-fired power plants.

The son of Russian Jews who met on a ship while emigrating to the United States in 1905, Weinberg was born April 20, 1915, in Chicago. He died October 18, 2006, in Oak Ridge at the age of 91.

The author of several books, numerous speeches and 541 scientific papers, Weinberg was a nuclear energy pioneer and prophet. He advocated the peaceful use of nuclear energy for producing electricity and medical radioisotopes. He also made accurate long-term predictions about energy technologies. He was a brilliant scientist and innovative scientific administrator. He was a thought-provoking communicator, coiner of words and a man of conscience and social responsibility who cared intensely about the welfare of humankind.

"Alvin was a worrywort for the human race," says his niece, Judith Goleman. In his last papers, authored in his late 80s, Weinberg was concerned about threats to humankind's survival—asteroids, nuclear waste, global warming and thermonuclear war— and capitalism's lack of compassion.

Weinberg was known on six continents. In Oak Ridge, this citizen of the world and Renaissance man was also a valued friend and neighbor. A lover of music and a musician, Weinberg played Bach preludes and fugues, as well as Christmas carols, on his Steinway grand piano and occasionally gave public concerts. Until his mid-80s he was a competitive tennis player with his backhand slice.

Early in life he followed in his sister Fay's footsteps, serving as editor of his high school newspaper. After earning B.S., M.S. and Ph.D. degrees from the University of Chicago, Weinberg was recruited at age 26 to help the Manhattan Project, started in 1942 to develop the atomic bomb.

In Chicago he performed calculations for his mentor and hero Eugene Wigner, a Hungarian theoretical physicist who designed plutonium-producing nuclear reactors at Hanford, Wash., and later won the Nobel Prize in physics. Other scientific giants of the 20th century with whom Weinberg worked, giving birth to the nuclear age, included Enrico Fermi, Leo Szilard and Edward Teller.

Weinberg headed the nuclear design of the Graphite Reactor at Clinton Laboratories in Oak Ridge, where he and his family moved in 1945. The "X-10 pile," the world's first continuously operating reactor, produced recoverable amounts of plutonium, paving the way for production of this fuel at Hanford to power the atomic bomb that ended World War II.

In 1946-47, when Wigner was research director at Clinton Laboratories, Weinberg developed his administrative skills, first as the physics division director and then as ORNL's research director in 1948, replacing Wigner. Weinberg is credited with saving the Laboratory from shutdown, convincing the federal government that ORNL had reactor development capabilities vital to the nation. In 1955 he was named ORNL director.

Of the books that Weinberg wrote, he was most proud of the work he coauthored with Wigner, entitled *The Physical Theory of Nuclear Chain Reactors*. "That's probably my most important contribution to science," he once told the editor of the *ORNL Review*, which he founded in 1967.

Weinberg was the first to publish and promote to key Navy officers the concept of the pressurized water reactor. The energy source for U.S. nuclear submarines became the dominant reactor design in commercial nuclear power plants, which today provide 16 percent of the world's electricity.

Freeman Dyson, renowned physicist with the Institute for Advanced Studies at Princeton University, writes in a 2006 letter that, in 1956, Weinberg taught him and others at General Atomic Company the particulars of nuclear reactor function and design. Dyson continues:

"Weinberg made ORNL the best place in the world for designing and building nuclear reactors. Oak Ridge developed the basic technology for scientific research reactors, electric power reactors and Navy submarine propulsion reactors. He was the only nuclear pioneer who supported the wide universe of reactor designs, going beyond the conventional solid-fueled reactors. He built liquid-fueled reactors with highly original designs."

Of Weinberg's broader influence at the Laboratory, Dyson writes: "His vision for Oak Ridge went far beyond nuclear reactors. He made ORNL become an outstanding international center for research in pure physics, chemistry and biology, as well as ecology and environmental science. He was interested in all kinds of energy technology and the effects of technology on the environment.

"Long before the subject of global warming became fashionable, he set up a research program in Oak Ridge to study the effects of carbon dioxide emissions on climate. This program trained many people who became leaders in climate studies at other institutions."

Alex Zucker, former acting director of ORNL, says Weinberg's leadership sprang from his interest in knowing ORNL researchers and understanding their work. "His trademark was sitting in the front row at information meetings and asking penetrating, and sometimes embarrassing, questions," Zucker notes. "If he approved—euphoria."

"The fundamental problem in the philosophy of scientific administration is the question of value." ***Alvin Weinberg***

Weinberg was a member of the President's Science Advisory Commission. In 1961 he chaired the Kennedy Administration's Panel of Science Information, which issued the report "Science, Government and Information." Also known as the Weinberg Report, it emphasized the need to communicate meaningful scientific information to technical and lay audiences.

A popular speaker and bold thinker, Weinberg coined new words to explain his groundbreaking ideas about energy and science to lay audiences. Examples are "burning the sea" (fusion), "burning the rocks" (fission), "nuclear-powered agro-industrial complex," "nuclear priesthood," "technological fix," "Big Science" (megaprojects like the moon mission), and the "Faustian bargain" for nuclear power. Weinberg started the annual "State of the Laboratory" address for informing the Oak Ridge community about ORNL research.

Weinberg left ORNL in 1973 and started Oak Ridge Associated University's Institute for Energy Analysis, which he directed from 1975 to 1985. IEA was the first organization to receive significant funding from the Department of Energy for climate studies. In 1974, he worked in Washington, D.C., as director of the U.S. Office of Energy Research and Development to help address the energy crisis. One of his office's recommendations, to establish a solar energy research institute, resulted in the creation of a DOE national lab in Colorado, now called the National Renewable Energy Laboratory.

Weinberg told the *Review* in a 1995 interview that his most important and original contribution was to develop criteria for measuring the value of competing scientific ventures. The National Science Foundation uses many of these criteria to guide funding decisions.

Weinberg was elected to the National Academy of Sciences, National Academy of Engineering, American Philosophical Society and American Academy of Arts and Sciences. He received dozens of honorary degrees. He won the Atoms for Peace Prize, Enrico Fermi Award, E. O. Lawrence Award, Hertz Prize and even the 1950 Young Man of the Year Award from the U.S. Junior Chamber of Commerce.

Weinberg promoted peace and the end of the nuclear arms race. He led the International Friendship Bell project in which two bronze bells manufactured by Japanese artists were placed in Oak Ridge and Hiroshima, target of the first atomic bomb. He advocated the "sanctification of Hiroshima" to make the Japanese city a permanent shrine against nuclear war and for the tradition of non-use of nuclear weapons. The American Nuclear Society, which he helped establish, awards a Weinberg Medal "for contributions to the understanding of the social implications of nuclear technology."

Weinberg's biggest disappointment was that he did not live long enough to witness the "second nuclear era" with inherently safe nuclear power reactors that would replace fossil fuel plants and curb global warming. ORNL—the multidisciplinary laboratory he rescued, built and personified—continues the effort to realize his dream.—*C. K.*

...and the WINNERS are...

Accomplishments of Distinction at Oak Ridge National Laboratory

At the annual UT-Battelle Awards Night, **Ian S. Anderson** received the ***ORNL Director's Outstanding Individual Accomplishment in Science/Technology Award*** for his exemplary performance in managing the installation of the Spallation Neutron Source target and instruments and for developing a strategy for the long-term success of the ORNL Neutron Science Program.

For his pioneering nuclear astrophysics studies, **Daniel Bardayan** received the Department of Energy's ***Presidential Early Career Award for Scientists and Engineers*** in a White House ceremony.

Steve Zinkle received the ***American Nuclear Society's 2006 Outstanding Achievement Award*** from the ANS's Materials Science and Technology Division for "sustained contributions to the understanding of metals and ceramics materials behavior for fusion and advanced fission reactor applications." The ANS-MSTD Literary Award went to **Thak Sang Byun** and **Kenneth Farrell** for "Plastic instability in polycrystalline metals after low-temperature irradiation." **Cecil Parks** has been named a ***fellow*** of ANS. **Nancy Larson** received ANS's 2006 ***Mary Jane Oestmann Professional Women's Achievement*** for her technical leadership in the nuclear data field.

Patti Garland received the the U.S. Combined Heat and Power Association ***CHP Champion Award***.

Thomas Thundat has been elected a ***fellow*** of the ***American Association for the Advancement of Science***.

David Cole has been elected a ***fellow*** of the ***Mineralogical Society of America***.

Ron Graves has been elected a ***Distinguished Fellow*** of the ***Society of Automotive Engineers***.

Hua-Tay Lin has been named a ***fellow*** of ***ASM International***.

Charles Forsberg and **Nageswara Rao** have been named ORNL's 2006 ***corporate fellows*** for career achievements in science and technology, performance and leadership. **Forsberg** pioneered the separation of actinide and rare-earth elements from acidic high-level waste solutions, provided leadership on nuclear waste management issues, and helped develop new reactor concepts. **Rao** is nationally recognized for his pioneering contributions in high-performance networking and multiple-sensor fusion.

James W. Lee and his team received the FuelCellSouth 2006 Crystal Flame Innovation Award for their research on genetically engineering algae to increase their efficiency in producing hydrogen.

Rongying Jin has been recognized as a "Rising Star" by *Women of Color* magazine.

Three technologies developed at ORNL have earned ***Excellence in Technology Awards from the Southeast Region of the Federal Laboratory Consortium for Technology Transfer***. The winners are **SeizAlert** for alerting patients and medical personnel of an epileptic seizure so that preventive action can be taken in time; **hybrid solar lighting**, a light system for rooms that uses natural sunlight combined with sensor-controlled artificial light during cloudy days and at night, and a **computer-designed methodology to produce steel alloys**. Earning honorable mention were ORNL's LandScan 2004 global population dataset and MEMS-based uncooled infrared imaging.

next issue

Energy Efficiency and Renewable Technologies

online extras

www.ornl.gov/ORNLReview

on the web

In Weinberg's own words:
Listen to thoughts of the late Alvin Weinberg in audio excerpts from interviews over the past decade. Plus, view a slideshow documenting Weinberg's life.

Jeremy Smith uncut:
Read an expanded version of the first Governor's Chair appointee's interview with the ORNL Review, including his comments on cultural differences, from science to soccer, in the various countries where he has worked.

Bioinformatics for bioenergy:
Learn about ORNL's software-based "bookkeeping operation" that will keep track of data, chemicals and experimental equipment for bioenergy researchers.

Reference desk:
View papers associated with the various research projects mentioned in this issue of the ORNL Review along with copies of the "Billion Ton" study and the DOE Biomass to Biofuels Workshop Summary: Breaking the Biological Barriers to Cellulosic Ethanol.

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