

OAK RIDGE NATIONAL LABORATORY

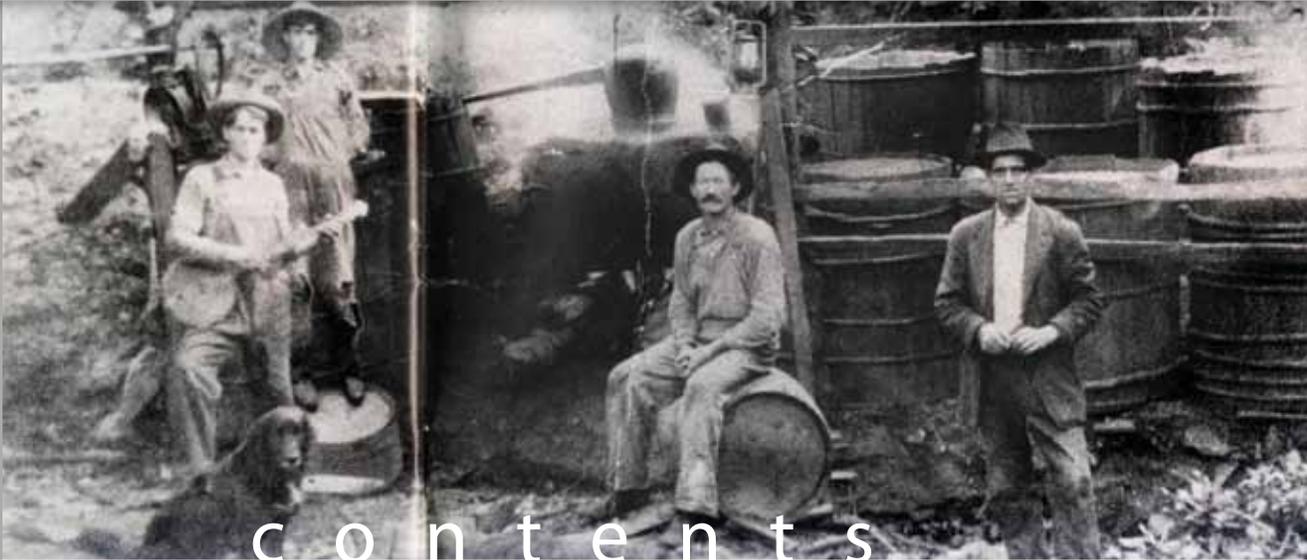
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REVIEW

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

The Next Generation of Biofuels

Sustainable Feedstocks
Cost-Competitive
Options



Photos courtesy of
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A Legacy Continues

On a clear day at Oak Ridge National Laboratory, one can see in the distance the Smoky Mountains, a spectacular range cloaked in green forest that defines Tennessee's eastern boundary. Since the late 18th century, the mountains have been home to families and individuals who have left an indelible mark on the culture of a modern society that today has largely passed them by.

If we know where to look, the legacy of our mountain ancestors can be found even in one of the world's most modern research laboratories. Visitors to the ORNL campus are often struck by the site of spectacular science facilities located adjacent to a small white wooden church. Now closed and maintained as a museum by the Laboratory, the New Bethel Baptist Church stands sentry by a picturesque graveyard, a reminder of those who lived and worked here generations before the Manhattan Project.

On the other end of the campus, another legacy of our mountain ancestors can be found amid the test tubes and laboratories, where scientists at the Department of Energy's BioEnergy Science Center are seeking to decode the mysteries of cellulosic ethanol. The irony of their work is inescapable. For more than 250 years, the people of the mountains around them have perfected what is essentially the same task—separating the sugars from plants to make alcohol. With little formal education and working with only the most primitive tools, the “moonshiners” produced a product that over time became a fundamental component of the Appalachian economy.

Today, equipped with state-of-the-art facilities and supported by some of America's leading scientific talent, ORNL's BioEnergy Science Center in many respects is attacking the same scientific challenges faced by our ancestors in the hills and hollows of the Smoky Mountains. For ORNL, the stakes are higher. Instead of producing alcohol for limited local consumption, the Laboratory has been assigned the challenge of helping decipher the evolutionary code for an entirely new generation of biofuels capable of transforming the American automobile industry.

Three years into this effort, this issue of the *ORNL Review* examines initial findings that have exceeded expectations. Researchers believe they are within reach of developing new enzymes and microbes that can not only breakdown the resistance of plants to sugar extraction, but do so in a way that produces biofuels at a cost competitive with that of gasoline. Equally important, they are using crops such as switchgrass and poplar trees that do not require the amounts of water, fertilizer and farmland that in the past have raised questions about the environmental sustainability of domestic biofuels as a viable replacement for imported oil. Perhaps most exciting, the quest to develop cellulosic biofuels also has incorporated potential uses for the byproducts of the manufacturing process. If these products, which include low-weight and high-strength carbon fiber, can demonstrate their commercial value, their economic potential is unlimited.

Meanwhile, these remarkable discoveries are a faint echo of days gone by, the legacy of a scientific challenge that endures in the hills of East Tennessee.



Billy Stair
Director
Communications and External Relations

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Director
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Commercializing Graphite Foam Technology

A new technology developed at Oak Ridge National Laboratory that extends the life of light-emitting diode lamps has been licensed to LED North America.

Signed at a ceremony with Lab Director Thom Mason, the agreement exclusively licenses a graphite foam technology developed by James Klett and colleagues of ORNL's Materials Science and Technology Division. LED North America will use the graphite foam to passively cool components in LED lamps, which are increasingly in demand for applications such as street and parking garage lighting. LED North America specializes in providing LED lighting products for municipal, commercial and industrial applications.

Because each 10-degree decrease in temperature can double the life of the lighting components, cooling LED lamps is critical to improving their efficiency. Using graphite foam to more efficiently dissipate the heat of LEDs is expected to extend their

lifespans and lower their costs, making the technology more attractive to a broader consumer base.

"While this technology will reduce temperatures and increase the life of the LED lighting systems, the greatest long-term benefit will be the cost savings to municipalities from reduced fixture replacement and maintenance," Klett says.

The newly licensed graphite foam invention offers a number of advantages over comparable heat sink materials, such as copper and aluminum. Graphite foam's high thermal conductivity, low weight and easy machinability offer the material greater design flexibility and provide a lighter, cheaper and more efficient cooling option.

The foam's well-ordered graphite structure is the key to conductivity. The manufacturing process produces a skeletal structure full of air pockets, leaving the foam lightweight and only 25 percent

dense. The network of ligaments in the foam wicks heat away from its source, providing an excellent candidate to cool the LED lamp components.

Championed as an energy saving lighting source, LEDs are expanding market share because of their lower energy consumption, compact size and longer life expectancy. Improved LED performance could enable LED North America to offer longer warranty periods than current competitors.

LED North America's relationship with ORNL was a factor in the decision by Andrew Wilhelm, one of the company's founders, to locate the company in Tech2020, an Oak Ridge high-tech business incubator.

"The proximity to ORNL provides us the opportunity to work closely with the Laboratory's researchers to further refine the integration of the graphite foam material into LED lamps," Wilhelm says.



Storming the Winter Palace

With the help of funding from the American Recovery and Reinvestment Act, ORNL's 1940s-era Quonset huts are in the final stages of demolition. Overlooking the laboratory's Oak Ridge Science and Technology Park, the aging structures were part eyesore and part historic reminder of ORNL's post-war role in the years following the Manhattan Project. Despite their historical significance, the buildings were simply too deteriorated to preserve.

The fact that the structures were Quonset huts suggests they were never intended to be permanent structures. Nonetheless, they were used for a variety of purposes over the years. In a humorous comparison to the opulent home of the Russian Czars in St. Petersburg, the rusting facilities became known as the "Winter Palace" when the UT-Battelle contract transition team used them for offices in the winter of 1999-2000.

The demolition of the structures will make available land for expansion of the adjacent Science & Technology Park, the first privately developed R&D park within the campus of a national laboratory. The



park is a key part of the redevelopment of the Manhattan-era section of the ORNL campus.

Lab Director Thom Mason says, "We felt it just didn't make sense to have one of ORNL's most dilapidated buildings only a

block away from some of the world's most modern research facilities."

ARRA funds were also used for the recent demolition of the Radioisotope Development Laboratory, which has been closed since the 1980s.

Park leads ORNL's Global Security



Brent Park has joined ORNL's Leadership Team as the new Associate Laboratory Director for the Global Security Directorate. Drawing on more than a quarter-century of experience in physics research and management, Park is well-positioned to lead the growth and integration of the laboratory's broad portfolio of security programs.

Park began his career in 1989 at Los Alamos National Laboratory, where he worked

as a postdoctoral fellow in the Physics Division and eventually rose through the ranks to become deputy director of the Nuclear Nonproliferation Division. He later served as the leader of the Homeland Security Technologies Division at the Nevada Test Site and as director of the Department of Energy's Remote Sensing Laboratory in Las Vegas.

In his new position, Park directs efforts to provide technical solutions to prob-

lems of national and global security. His new directorate specializes in the detection, prevention and reversal of the proliferation of weapons of mass destruction. The group's activities include international efforts to help secure nuclear materials, improving safeguards and security systems and providing accounting systems that track the location of nuclear materials.

IT MIGHT JUST HAPPEN

An interdisciplinary approach could unlock the secrets of cellulosic biofuels.

The scientific challenge is straightforward. If the U.S. hopes to realize significant reductions in both the volume of imported petroleum and the level of carbon emissions, a portion of the solution will involve a substantial increase in the use of biofuels by the domestic automobile industry. The willingness of Americans to embrace biofuels, and the subsequent economic transformation in a variety of industrial sectors, will depend in large measure on whether researchers at Oak Ridge National Laboratory can find a way to produce cellulosic ethanol at a cost that is competitive with that of gasoline.

At the midway point of a five-year mission to revolutionize the production of biofuels, ORNL's BioEnergy Science Center (BESC) has made considerable progress toward overcoming several fundamental scientific roadblocks. One key to this progress is BESC's unprecedented coalition of industrial, academic and government partners that has made possible an interdisciplinary

approach to research and development. Associate Laboratory Director for Biological and Environmental Sciences Martin Keller has the daunting task of coordinating the partners and integrating a variety of laboratory research functions as diverse as land use planning, biomass conversion and the linkage of bio-based products, such as lignin carbon fiber, to biofuel production. Prior to his promotion in February 2010 to associate lab director, Keller served as the director of BESC. The center's new director is Paul Gilna, who has assumed the role of managing the multifaceted system of partnerships and collaborative research efforts for the Department of Energy. Keller is quick to point out that because the problems addressed at the center are both interconnected and broad in scope, BESC's research efforts, by definition, must be interdisciplinary. While the center's research targets are guided by DOE, Keller and Gilna are working to leverage BESC's capabilities with other bioenergy projects across ORNL.



Sustainable crops

The first consideration for any bioenergy production effort is the sustainability of the “feedstocks,” or crops, on which the process relies. “If we look back at what happened when corn-based ethanol became popular,” Keller says, “few researchers paid enough attention to issues of sustainability.” He stresses that the practical limits of feedstock production, land use changes, environmental impacts and the effect of feedstock production on the price of food need to be resolved before America can establish a sustainable biofuels industry. “The questions we ask now will have an impact on the project’s ultimate success,” he says.

If large-scale biofuel production can be established and sustained, Keller envisions an economy in which as much as 30 percent of the energy required for transportation would come from biofuels. He also anticipates that a significant

percentage of the steel used in cars could be replaced by lightweight carbon fiber, a biomass byproduct. Keller says answers to a number of fundamental sustainability questions were provided by the “Billion-ton Study,” which concluded that the U.S. could produce a tremendous volume of biomass. “We now need to go a step further and determine in what specific areas we can grow these crops, which crops should be grown where and whether these feedstocks will require a change in our agricultural practices. All of these questions are being considered by ORNL’s Center for BioEnergy Sustainability.”

Better plants, better enzymes

As they sort through sustainability issues, BESC scientists are also investigating “recalcitrance,” the most intractable problem facing the biofuels process. Recalcitrance is the term researchers use to describe the difficulty of extracting the sugars stored in the stalks, branches, and stems of plants. Producing biofuels involves converting plant material into accessible sugars and then fermenting those sugars into biofuels, such as ethanol. “Nature made plants extremely resistant to this process,” Keller explains. “The

We envision an economy in which as much as 30 percent of the energy required for transportation would come from biofuels.

Passing Milestones

ORNL’s BioEnergy Science Center opened in 2007. Over the past three years the new program has passed a number of major milestones—many ahead of schedule. Perhaps the center’s most critical milestone was the ability to use molecular biology to make plant cell walls easier to break down into their component sugars. While much remains to be done to refine the process, ORNL’s Associate Laboratory Director of Biological and Environmental Sciences Martin Keller says the milestone has essentially been reached. He notes that BESC scientists thus far have discovered two exceptional switchgrass lignin genes with the ability to reduce the amount of lignin produced by switchgrass, increase its ethanol production and reduce the amount of enzyme needed to sustain the process. “These new plants are growing in a greenhouse right now and will be planted in field trials next year,” Keller adds. Having shown the proof-of-concept with these genes, the next challenge is to test additional genes and understand their impacts. More genes targets have been modified, and the testing of the resulting plants has begun. Reaching this milestone demonstrates that the process of producing biofuels from biomass can be made much more efficient and that the cost of conversion can be significantly lowered.

Another of the center’s major milestones was proving that consolidated bioprocessing—a one-step process for converting biomass into ethanol—could work. Keller says that Mascoma Corporation, one of BESC’s partner organizations, is close to demon-

strating that a specially modified strain of yeast can reduce biomass to sugars and ferment the sugars into biofuels in one step. “This is an area in which we have made significant breakthroughs and where we are far ahead of schedule,” he says.

Despite the progress, significant challenges remain, such as understanding how various plant cell wall components interact on a chemical level, including how cellulose, hemicellulose and lignin are linked at the molecular level. The challenge has implications for the relative difficulty researchers may encounter in extracting sugar from biomass. Data from recent studies on various molecular interactions have provided hints about which aspects of cell wall structure can be modified to make them easier to break down, allowing sugar to be extracted more efficiently.

Another milestone will be to demonstrate a synergy among the center’s advances on a variety of scientific fronts. BESC researchers know, for example, that modifying plant cell walls can boost the efficiency of biofuels production and that consolidated bioprocessing is expected to provide a similar increase in efficiency. Still unknown is whether, if the two techniques are combined, the resulting efficiency increase would be greater than expected.

“We want to know if two plus two can equal five,” Keller jokes. Given his insistence that the whole is greater than the sum of its parts, the question remains open.

complexity of the conversion process is the primary reason the biofuels industry has not taken off." The three major components of biomass are cellulose, hemicellulose, and lignin. BESC researchers are searching for both a cost-effective way to separate the lignin from the cellulose and hemicelluloses and an equally effective way to digest cellulose and hemicellulose into sugars and ferment them into biofuels. Keller says that BESC scientists are trying to understand, at the biochemical and genetic levels, why biomass is so hard to digest. Once they unlock this door, the equally important challenge will be to identify or engineer new enzymes and microbes to make the digestion process cost effective.

In the quest for better biofuel feedstocks, BESC scientists are also developing microbes with unique capabilities to break down biomass into its component sugars. "We know that if we cut down a tree in

the forest, it will lie on the ground and eventually decay and disappear," Keller says. "The tree will ultimately be digested; it just takes a long time. In a similar way, our goal with biomass is to accelerate this process." To gain a more detailed understanding of exactly how plants are decon-

structed by microbes, BESC researchers are designing computer simulations of plant cell wall structures. Their goal is to determine where and how to make genetic modifications to these structures that would render them easier to digest. "BESC is bringing together an unprecedented



consortium of 20 institutions and the collective resources of molecular biologists, biochemists and computer scientists to overcome this fundamental problem of recalcitrance,” Keller says.

Broadening the research base

Another major focus within BESC’s biofuels program is integrating biological studies focused on creating better plants and enzymes with research being done by chemical and materials scientists on separating various constituents within the biofuels production process and catalyzing the chemical reactions. Keller says ORNL benefits from a history of effective separation technologies research. “By bringing the laboratory’s separations scientists into the collaboration, we have been able to apply their knowledge and experience to the challenges posed by bioenergy.” The collaboration plays a critical role in increasing the pace of BESC’s efforts to combine the pretreatment of biomass and the separation of its key components,

such as cellulose and hemicellulose, into a single, continuous process.

The laboratory also has considerable expertise in catalysis, a process that involves starting or accelerating chemical reactions. One area in which this expertise is being applied is biofuels fermentation. Ideally, BESC will eventually be able to produce not just ethanol, but also other biofuels that are more compatible with America’s current fuel supply. To accomplish this, researchers will need to do one of two things. They must either modify the microorganisms to enable them to ferment sugars into fuels with longer-chain carbon molecules or devise a chemical means of converting the ethanol produced by these organisms to higher hydrocarbons—or a combination of both techniques. Understanding the chemical pathways by which these higher hydrocarbons can be produced is critical to success. “This scientific challenge explains why we are integrating catalysis specialists into the research process,” Keller says. “Traditionally, scientists in different disciplines

might have investigated the problem from isolated bubbles. Our success has come in part from bringing people together across disciplines.”

As additional biofuels are developed, Keller is accessing the resources of the National Transportation Research Center, where ORNL researchers are testing various biofuel blends to determine emission and efficiency performance in a variety of engines. This capability will become increasingly important as biofuels are created that can be introduced directly into the current energy infrastructure. The center’s researchers also model combustion, applying their findings to studies of biomass combustion for both gasification and power. Gasified biomass (or syngas) can be converted into fuels through catalysis or fermentation, yet another illustration of interdisciplinary research in the bioenergy arena.



ORNL researchers gather microorganisms to aid in biomass conversion from Yellowstone National Park’s hot springs.



Valuable leftovers

Lignin, or plant fiber, accounts for most of the leftover material after the sugars have been extracted from biomass. In a conventional biomass conversion process, this leftover fiber would be burned to create heat for other processes, such as producing steam used to generate electricity. This particular bioenergy byproduct, however, has a higher value potential. With funding from DOE's Office of Energy Efficiency and Renewable Energy, ORNL is promoting a more efficient approach that involves converting lignin, the biofuel byproduct, into carbon fiber for use in lightweight automotive and aircraft components. Keller predicts that if lignin could be used to create carbon-fiber components that are cost-competitive with steel, the material's low weight and high strength would quickly generate a market in an automobile industry constantly in search of better fuel mileage. "If we could replace a significant portion of the steel in a car with carbon fiber," Keller reasons, "the car would be

much lighter, require less fuel, and, in turn, reduce the demand for imported oil. Fuel efficiency must go hand-in-hand with biofuels. We cannot simply replace one kind of fuel with another. In order to create a sustainable model, we have to deliver fuel efficiency, as well."

Bridging islands of science

Keller stresses that, while the pressure for breakthroughs in the field of biofuels production is undeniable, the keys to success are communication and cooperation across scientific disciplines and among organizations. The need is too pressing, the questions too broad and the problem too complex for any single group of scientists. "We're trying to get researchers to look at the problem of providing energy for transportation in an integrated way. If we want to succeed, if we hope to create a sustainable biofuels industry, we cannot remain islands of science. The only path forward is an integrated approach to addressing one of the most important scientific challenges of our lifetimes." 

TWO STEPS FORWARD

The path from biomass to biofuels just got shorter.

One of the primary goals of ORNL's BioEnergy Science Center (BESC) is to revolutionize the processing and conversion of biomass into biofuels, such as ethanol. A critical component of this revolution is the capacity to streamline the bioconversion process and optimize its outputs, a goal shared by Ramesh Bhave and his colleagues in ORNL's Materials Science and Technology Division as they continue on the path toward developing an unprecedented method of combining the pretreatment of biomass and the separation of its key components into a single, continuous process.

"The vision of the bioenergy center is to find innovative ways to convert biomass into fuels," says Bhave. One of the key steps in this process is to develop an effective pretreatment technique, one that breaks down the biomass effectively, making it more amenable to biochemical conversion and increasing its yield of sugars and other chemicals that might be of value.

"This is where our group's expertise in the area of separations technology becomes important," Bhave says. "Developing the ability to effectively separate sugars and other biomass components could accelerate bioconversion." With that goal in mind, the efforts of Bhave's group are focused on a unique pretreatment regimen for the conversion of biomass to fuels using very selective, robust membranes that can operate under harsh pretreatment conditions, enhance the yields of the sugars and minimize byproducts that decrease the efficiency of the process.

Bhave believes that the breadth of talent represented by BESC's academic and institutional partners has been critical to the project's early success. "We are working with Dartmouth College because it is a leader in researching and understanding pretreatment," he says. "Dartmouth's engineering department has studied biomass pretreatment technologies for thirty-plus years." When the Department of Energy established BESC, Dartmouth became a

very desirable research partner because its pretreatment expertise, combined with ORNL's capabilities in the area of chemical separations, enables us to make the separations process more effective and more efficient at a lower cost."

Bhave characterizes consolidated bioprocessing as a question of how biomass can be pretreated so as to become more amenable to biochemical conversion and



Membranes that can withstand harsh pretreatment conditions are used to streamline the biofuel production process.

produce more of the products, like sugars, that will increase the yield of biofuels. “If we look at the problem from that perspective,” he says, “separating the products released by pretreatment becomes an important part of the process. If we could develop effective separations methods, they would assist in the bioconversion process.”

Toward that end, Bhavé and his colleagues are working on a novel pretreatment process for biomass conversion. The key to the process is the use of selective filter membranes that can operate under very aggressive pretreatment conditions. The ability to extract various biomass components, such as sugars, proteins and lignins, while the biomass components are still in the pretreatment environment, enables researchers to boost their yields. This increase occurs because, in a continuous process, the components spend less time in the harsh preprocessing environment and are, therefore, less likely to break down into other compounds.

The pretreatment process begins with small chips of plant material from energy crops, or “feedstocks,” such as switchgrass. “The process could be applied to a range of feedstocks,” Bhavé explains. “What we are looking for in the various energy crops is a cell structure that is less resistant to pretreatment, so the sugars can be released from the biomass using less energy and fewer chemicals.” This feedstock is pretreated to break down its cell structure, which releases liquid containing

various chemical products, including the sugars needed to produce biofuels. This process typically requires the use of moderately high temperatures, along with dilute acids or bases.

At this point in the traditional pretreatment process, the liquid would be left to cool so the solubilized products could “precipitate” or separate from the liquid. In Bhavé’s process, a flowing water stream interacts with the heated biomass, carrying away organic components that contain sugars and other soluble products released by pretreatment. This is where the laboratory’s separations expertise comes in. At this point, the dissolved material is retained by the membranes that are designed both to withstand the aggressive pretreatment environment and to separate sugars and other organic components that have been released by the biomass. One of the advantages of this integrated approach to preprocessing and separation is that it potentially minimizes the time the biomass is in the harsh pretreatment conditions. This, in turn, would minimize the production of materials, such as degraded sugars, that could stop the fermentation process.

“This all happens under pretreatment conditions,” Bhavé emphasizes. “We don’t wait for things to cool down. In the pretreatment process, the components are basically just dissolved at high temperature. If the pretreated biomass were allowed to cool down, its dissolved compo-

nents would precipitate into solids.” Once this occurs, a much more difficult and energy-intensive chemical process would be required to recover the sugars from the other components, he says. “Separating sugars and other components from the rest of the biomass during pretreatment is an approach that, to our knowledge, has not been taken before,” Bhavé says. “It requires an understanding of both the pretreatment process and the ability to apply membrane separation technology in an entirely new way.”

As they work to fine-tune the separations process, Bhavé and his colleagues are addressing the challenge of creating membranes that have multiple functions. “We need membranes to do the separation, withstand the preprocessing conditions and be able to be regenerated, or cleaned, periodically,” he says.

The ability of Bhavé’s team to consolidate separations technology using the pretreatment process suggests that BESC is making significant strides in the processing and conversion of biomass. Bhavé isn’t yet predicting a revolution, but he is excited by the project’s potential. “The research is promising,” he says, “but it is also challenging. We are hopeful that the price of the biofuel produced by this process will be lower because our pretreatment costs and energy costs are lower.” Perhaps more than Bhavé realizes, his hopes are shared by a nation increasingly eager for low-cost alternative fuels. **R**

SUGAR-COATED

Researchers are closing in on new ways to separate sugars needed for biofuels.

Oak Ridge National Laboratory's BioEnergy Science Center (BESC) was established in 2007 after a spirited competition by the Department of Energy's Office of Biology and Environmental Research to conduct fundamental research related to biofuel feedstock development, cellulosic ethanol production and investigations of the plant and microbial enzyme components of the biofuels production process. "The center's basic premise," says BESC Director Paul Gilna, "was to develop an improved body of scientific knowledge and understanding to underpin the production of biofuels from plant sources and, in so doing, to harness that knowledge to develop strategies that would significantly improve the process of generating biofuels."

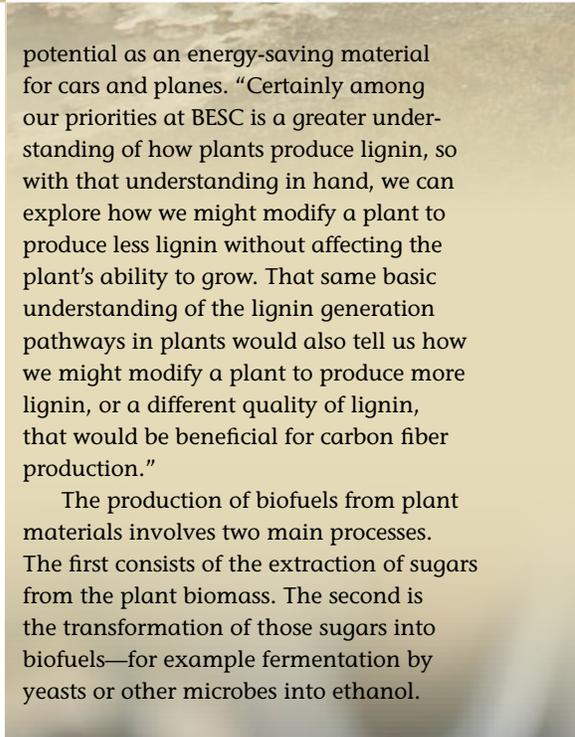
Most of the plant material currently used to produce ethanol in the U.S. is the starchy part of corn. The use of corn for ethanol production, both domestically and abroad, raises serious questions about using food crops and valuable farm land for the production of biofuels. BESC's research efforts are designed to look more closely at the sugars trapped in other plant structures, as well as other plants, that could be used to produce biofuels. Plant parts such as stalks and leaves are composed of fibers made from complex carbohydrates, such as lignin, that in turn contain cellulose. Like kernels of corn, they also contain sugars that can be used to produce biofuels. Unlike corn, the structural complexity of the fibers makes the sugars more difficult to separate. If scientists can unlock the secret to extracting these sugars quickly and cheaply, they can be adapted to the same manufacturing processes currently used to generate ethanol from corn.

In one sense BESC has a single goal—to overcome "recalcitrance," a characteristic that some describe as nature's way of protecting a plant by making it difficult to access the simple sugars in the complex carbohydrate fibers in which they are bound. Once separated, these sugars are available for the production of ethanol and other biofuels. "If we can solve the puzzle of recalcitrance," Gilna says, "we can open up avenues for more efficient production of biofuels and do so in a way that does not compete with the production of food. In fact, in some cases we would be taking advantage of the waste stream of food production, like discarded cornstalks, to produce biofuel. In other cases, we could use feedstocks such as switchgrass or poplar trees that do not compete with land used for food crops." BESC scientists are looking at a variety of potential feedstocks, with an emphasis on those that do not compete for agricultural land. In particular, they are seeking crops that can be grown in more arid climates and in rotation with food crops to complement existing agricultural practices. The broader goal is to develop a diversity of biomass feedstocks for the next generation of biofuels that require less water and fertilizer and can be grown on marginal land.

As BESC researchers succeed in breaking down recalcitrance in plant material, they open up the possibility of using a number of compounds stored in plants, besides sugars, for the production of other products and chemicals. One commonly cited example is lignin, the fiber that helps plants stand up. Colleagues at ORNL are excited about the use of lignin as a raw material for producing carbon fiber, a compound which is lighter but stronger than steel or aluminum and has enormous

potential as an energy-saving material for cars and planes. "Certainly among our priorities at BESC is a greater understanding of how plants produce lignin, so with that understanding in hand, we can explore how we might modify a plant to produce less lignin without affecting the plant's ability to grow. That same basic understanding of the lignin generation pathways in plants would also tell us how we might modify a plant to produce more lignin, or a different quality of lignin, that would be beneficial for carbon fiber production."

The production of biofuels from plant materials involves two main processes. The first consists of the extraction of sugars from the plant biomass. The second is the transformation of those sugars into biofuels—for example fermentation by yeasts or other microbes into ethanol.





In addition to understanding the recalcitrance of feedstocks, Gilna's staff also wants to improve the fermentation process. Researchers have identified a variety of fungi and other microbes that digest the sugars bound up in the complex carbohydrate structures of plant material. Wood rot, largely the product of a fungus, is one such example. Similarly, BESC scientists have discovered thermophilic, or heat-loving, bacteria that live in the hot springs of Yellowstone National Park that also can digest cellulose.

Gilna is convinced that science has much to learn from these microbes and fungi. As a result, his team is expending considerable effort studying microbes that have developed the ability to degrade or digest cellulose and lignin for their own needs. "If we could understand better the enzyme pathways that are responsible for

this degradation, we could then engineer these pathways into the strains of yeast and microbes that are used in industrial fermentation processes." Looking ahead, scientists would like to identify or engineer microbes that could digest and ferment plant material in a single step, thereby reducing the cost of the resulting biofuel. One of the major drivers behind the Department of Energy's investment in BESC is the desire to promote increased use of biofuels in the domestic market by reducing the cost of production. "If biofuels are not cost-competitive, there will never be much demand," Gilna concludes. "We have to find strategies that will lead to cost reductions."

The search for a better fundamental understanding of the science surrounding biofuels production and an opportunity to apply this understanding to America's

transportation sector lie at the heart of BESC's efforts to develop affordable, sustainable biofuels. "There's a huge amount to be learned," Gilna says. "As we overcome the fundamental challenge of recalcitrance, we can move forward and continue to increase our understanding of the entire process."

One measure of this project's importance is the scale of resources dedicated to the task. BESC is one of three Department of Energy bioenergy research centers, each funded at approximately \$125 million, which encompass the efforts of about 1000 scientists working on the challenge of producing sustainable biofuels. Reflecting on the magnitude of the endeavor, Gilna says. "When is the last time we rallied together 1000 scientists for a problem like this? Some would say not since the Manhattan Project." 



FINDING A PATH

Researchers are closer to finding a catalyst to develop a cost-efficient biofuel.

Chaitan Narula, a senior scientist in ORNL's Materials Science and Technology Division, at times appears to be consulting a mental roadmap as he evaluates the various chemical routes available to turn biomass into a viable transportation fuel. He notes that some options produce byproducts that have no market and that others are not economical. Still other processing options yield fuels that do not perform well in the fuel distribution system or in existing vehicles.

The starting point for creating fuel from biomass is the output of biomass fermentation: a stream of liquid that is approximately seven to ten percent ethanol mixed with water. While this dilute stream could be distilled to pure ethanol and used as a fuel, the energy required and the compromise in engine performance make the option unattractive. The challenge for

Narula's research team is to devise a way to convert the ethanol directly to higher hydrocarbons using a catalytic process. The advantage of producing a hydrocarbon-based biofuel is that higher hydrocarbons (fuels based on more complex arrangements of carbon molecules) can be blended directly into existing supplies of gasoline and diesel fuels and used in existing vehicles. Equally important, they provide vehicles with the same amount of energy as traditional transportation fuels.

Previous attempts to convert ethanol to hydrocarbons have not been chemically straightforward. Narula describes one such process that starts with ethanol (an alcohol), converts the ethanol to ethylene (a hydrocarbon) and then to methanol (an alcohol), resulting in yet another hydrocarbon that can be mixed with diesel fuel.

"There is no economic reason to convert a hydrocarbon to an alcohol and back to a hydrocarbon," Narula says. "The energy required for these conversions makes these paths unfavorable."

The goal of Narula's research is a process that would produce such a fuel by passing a stream of dilute ethanol through a catalyst, a process similar to that of exhaust gases

moving through the catalytic convertor on a car. When the ethanol encounters the catalyst, a chemical reaction occurs, converting the ethanol to hydrocarbons. The hydrocarbons are separated from the water, and the water is recycled. Narula's team has completed preliminary work using a hydrogen zeolite catalyst, successfully converting a dilute stream of ethanol into ethylene, a simple hydrocarbon. The team is planning similar studies on metal catalysts. Both experimental evidence and computer simulations suggest that this approach could enable them to convert ethanol to higher hydrocarbons.

"The metal we will start with is iron," Narula says. "There is evidence from previous studies that, when iron is added, the zeolite catalyst will interact with ethanol to produce higher hydrocarbons." Among the first challenges for Narula's team will be demonstrating that a dilute stream of ethanol can, in fact, be converted to higher hydrocarbons using the catalyst. If successful, the next step will be to find the catalyst that produces the best biofuel output. "The basic catalyst we are currently working with is just one of hundreds of zeolites," Narula observes. "There are many different metals that might be used in conjunction with the catalyst. Given the volume of potential metals, we want to proceed systematically, and not by trial and error."

The use of computer-based theoretical simulations is enabling Narula's team to narrow the field of possible catalysts from thousands of possible configurations to a handful that holds the greatest potential for success. "Our timetable does not have the years required to examine every possible catalyst," Narula says. The team believes that a combination of logic and careful experimentation will point to a pathway that produces a conversion of ethanol to hydrocarbons. Starting from that point, the team is trying to understand how the reaction works and, based on that understanding, improve the catalyst.

Simulations on ORNL's high-performance computers also enable Narula's team to examine the mechanics of how these ethanol-catalyst chemical reac-

tions occur by considering the structure of various zeolite catalysts and the structure of ethanol. This analysis helps them identify potential chemical pathways between ethanol and various higher hydrocarbons. In the case of their iron-zeolite catalyst, the researchers intend to evaluate the possible ways in which the catalyst can interact with ethanol, identify the potential intermediate steps along the way to producing higher hydrocarbons and calculate the most energetically favorable method of converting biomass to energy. Once they have identified a pathway, they will seek experimental confirmation of the intermediate chemical steps suggested by the simulation. The process's final steps will include additional simulations designed to improve the efficiency of the reaction and

increase the quality and quantity of the hydrocarbons produced.

Having found a potential pathway from ethanol to hydrocarbon fuel, the next part of their journey has begun. As the process of creating affordable, efficient hydrocarbon biofuels from biomass becomes increasingly viable, Narula says his team is now in search of an ideal catalyst, one that is superior to those that are currently commercially available. "We are developing some new catalysts in response to what we have learned from our simulation work and experimentation. We know it can be done. Our goal now is to improve our understanding of the reaction so we can develop a catalyst to optimize the process." [®]

Narula's team hopes to produce hydrocarbon biofuel by passing a stream of dilute ethanol through a catalyst.



A PREDICTABLE CHANGE

A new technique can change a plant's characteristics to make biofuels.

A core objective of ORNL's BioEnergy Science Center is to find ways to wring more energy out of the sugars stored in plants. In addition to developing better enzymes, improved microbes and more effective catalysts, Gerald Tuskan's team of plant biologists is exploring ways to generate more energy from biomass by "persuading" plants to store more sugar and then developing new methods of extracting these sugars.

Most of the sugar found in biomass is stored in plant cell walls as cellulose and hemicellulose. The biggest roadblock to extracting sugar from these cell wall polymers has been the difficulty of using biochemical tools to break down the walls. Tuskan, a scientist in ORNL's BioSciences Division, is working with a dozen Oak Ridge scientists and university collaborators to study the genome of *Populus*, a group of trees commonly used in both biofuels research and biofuels production. The team is seeking to determine which of the plant's 42,000 genes play a role in the formation of the cell wall and which of those can be modified and regulated to create cell walls that are more easily broken down. "It's important to note that we're not talking about placing 'foreign'

genes into *Populus*," Tuskan says. "We are modifying native genes that make it easier to break down the cell walls. We want to learn when these genes are turned on, how long they are on, and which plant tissues they are associated with."

Subtle changes

Currently Tuskan and his colleagues have narrowed to about 3580 the list of genes that might play a role in cell wall formation. They employ a variety of molecular techniques to study the genes and determine their respective functions. One of these techniques involves randomly inserting genetic "on" switches into the plant's genome to determine the effect. "Whatever gene the switch lands next to is turned on," Tuskan says. "We are inserting as many 'on' switches as possible to identify the function of as many genes as possible."

In about one quarter of the experiments, the technique produces a measurable change in the plant's physical characteristics. While some changes, such as coloration, are obvious to the naked eye, many are harder to discern. "The changes usually involve more subtle characteristics, like the level of sugar poly-

mers in the plant's stem," Tuskan says. To detect these changes, Tuskan's team grows modified plants and then analyzes both their chemistry and their outward appearance. When a change is detected, researchers examine the plant's genome, locate the newly inserted "on" switches, and determine which gene or genes the switches have activated. The approach provides scientists with a good idea of which genes produced the changes. Once they know what a particular gene controls and whether it appears to play a role in the formation of the cell wall, researchers can make an informed decision about whether the gene should be turned "on" or "off" to improve the plant's usefulness for producing biofuels.

One of the challenges the team is addressing using this "on" switch technique involves disentangling the relationship between the molecules of cellulose and hemicellulose; polymers that make up the plant's cell walls; and lignin, a polymer that provides strength and stiffness to the plant's stalk. The standard biofuels pretreatment process involves relaxing the bonds between the cellulose and hemicellulose cell walls and lignin using a combination of high tempera-

tures, dilute acid, and high pressure, so the lignin can be removed. Because the plant sugars are contained in the cellulose and hemicellulose, pretreatment removes the lignin but also has the undesired consequence of degrading the cellulose and hemicellulose, reducing the amount of stored sugar that can be captured.

In search of a process that removes lignin from the biomass without sacrificing sugars, the team is looking for genes that can control the degree of polymerization of both lignin and cell walls. A more highly polymerized molecule has a more complex structure that tends to bind tightly to neighboring structures, making it more difficult to break down. This quality is known as recalcitrance. For the purposes of biofuels research, scientists would like to reduce the lignin's polymerization to facilitate its separation from the plant's cell walls. At the same time, researchers are seeking to increase the polymerization of cellulose and hemicellulose to enhance resistance to degradation during pretreatment. "Our basic goal is to reduce the recalcitrance of lignin and increase the proportion of intact cellulose," Tuskan

says. "All of our genetics work is being driven toward those two goals."

Selective breeding also plays a role in the team's efforts to develop an optimized strain of *Populus*. Drawing on the biochemical analysis of the 1100 genetically different trees in their collection, the researchers found that *Populus*'s native lignin and sugar content vary greatly. "We have four individuals out of this collection that yield 87% of their theoretical maximum for sugar yield without any pretreatment at all," Tuskan says. "These are individuals we intend to either put in a breeding program or use for gene regulation research to determine the genetic basis for their favorable genetic characteristics."

Part of a process

A large part of what Tuskan and his team are trying to achieve is driven by the neighboring steps in the biofuels development process. Before they consider what kind of biomass would be suitable for producing biofuels, Tuskan and his colleagues have to examine issues of agronomy and sustainability. "The plants

must be efficient in how they use water, nutrients, carbon and space. They need to be able to grow in a wide range of areas in a way that does not deplete the soil of key nutrients. We also want to be sure that farmers can grow these biomass crops in an economically sustainable manner."

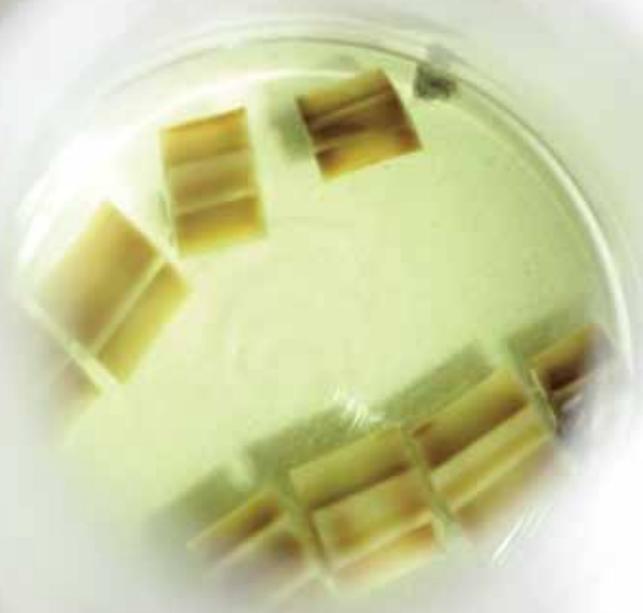
Similarly, much of the selective breeding and genetic fine-tuning Tuskan and his colleagues perform is aimed at making sure their final product has the sugar release, deconstruction and fermentation characteristics needed by the microbiologists who will be converting the plants to biofuels. "Our industrial collaborators are the ones most concerned with producing a sellable product," Tuskan explains. "Their short-term target is ethanol, but they are moving quickly toward higher-chain alcohols, like isobutanol or octanol. These fuels are preferable to ethanol because their energy per unit volume is similar to that of gasoline; they do not react with water; and they can be blended with gasoline in the current fuel distribution system."

Tuskan notes that when his group passes along a suitable feedstock to the bioconversion researchers, the process does not necessarily end. "We'll hear from them how well the biomass actually performs in the production process. We know how we expect the main polymers, cellulose, hemicellulose and lignin to perform, but there are other compounds in plants that can inhibit the biofuels production process. Before we know if we have a successful feedstock, we will have to see how it performs in an actual bioreactor."

"We hit the ground running"

Looking back at what has been accomplished by the BioEnergy Science Center in a relatively short time, Tuskan believes the center has made remarkable progress. "We really hit the ground running at BESC. Because we put an infrastructure together in a timely way, all the experiments are up and running. Usually with a project this size, there's a longer learning curve and a slow scale-up, but because of our team's experience and the quality of the participating institutions, we have exceeded our project milestones. Everything is in place for a period of genuine discovery." 

Scientists are generating more energy from biomass by studying the *Populus* genome.



New biofuels must be compatible with America's existing transportation infrastructure.

BUT ARE THEY COMPATIBLE?

The ultimate goal of ORNL's BioEnergy Science Center is, naturally, to produce biofuel—but not just any biofuel. To achieve the center's goal of helping to reverse the nation's dependence on oil imports, a successful biofuel will need to be a stepping stone that fits neatly into America's current fuel infrastructure as part of a path to a transportation system that rests far less heavily on petroleum products.

The research performed by Distinguished Scientist Bruce Bunting and his colleagues at ORNL's Fuels, Engines and Emissions Research Center (FEERC) focuses on ensuring that new biofuels meet both requirements. The research, funded in large measure by the Department of Energy's Office of Energy Efficiency and Renewable Energy through the Vehicle Technologies Program, is coordinated with the Office of Biomass Programs. The studies include the evaluation of biofuels for compatibility with existing cars and trucks, as well as with fuel production and delivery systems. Bunting explains that the transportation fuel infrastructure in the U.S. is made up of refineries, product pipelines, terminals that store fuel locally and trucks that transport fuel to service stations and trucking depots. "That system," he says, "has evolved over much of the last century to handle petroleum products, and does

an excellent job of providing high-quality, reliable fuels. The easiest way to adapt biofuels to this system is to make them as similar as possible to the existing petroleum-based fuels.”

FEERC scientists evaluate new fuels from a variety of sources, including those made by the BioEnergy Science Center, to determine whether they meet industry standards and to evaluate their impact on engine performance. They also provide feedback on chemical factors that improve engine performance and the compatibility of new biofuels with existing fuels. The process of testing new biofuels usually follows a similar pattern. Once the biofuel is blended with standard gasoline or diesel fuel, FEERC researchers analyze the mix to ensure that the blend meets industry standards for fuel quality. The fuel is then run in a highly instrumented laboratory engine to determine whether it meets performance expectations. Finally, the new fuel may be tested in conventional vehicles.

The majority of biofuel currently being produced is ethanol. Unlike gasoline, ethanol mixes easily with water, which can cause problems if it enters a vehicle’s fuel system. Because water is present at various points in the fuel distribution infrastructure, fuel companies keep ethanol and water separated by transporting ethanol to fuel terminals and blending it with gasoline late in the distribution process, literally as fuel trucks are loaded at the terminals. One potential alternative to using ethanol as a biofuel would be to make ethanol and then chemically convert it to hydrocarbons. Not only would this process help avoid water-related problems, but the hydrocarbons could be blended with gasoline or diesel fuel directly at the refinery. Because both gasoline and diesel fuel are blended from a variety of components, Bunting expects that successful biofuels will mimic one or more of these components and be blended into the fuel in a similar way. He notes that producing biofuels with higher octane (for gasoline) or cetane (for diesel) values might be the most effective approach because the components are worth more per gallon, making them more attractive to fuel producers. “Our goal,” Bunting says, “is to

use this process to replace about 20 percent of the nation’s petroleum-based fuel consumption over the next ten years”.

While Bunting discourages the idea of an undiscovered magic bullet that would revolutionize transportation fuel production, he does identify potential improvements that he views as realistic. “New fuels have to meet a number of requirements,” he says. “Most importantly, they must be compatible with existing vehicles. They also need to be compatible with the distribution system. And of course, biofuels must attract enough interest from the investment community to make them commercially viable.” Improvements seen by the consumer, he suggests, are likely to be gradual, making it easier to meet regulatory requirements and allowing a skeptical public to gain confidence in the new fuels.

Bunting expects the development of improved biofuels to be accompanied by improvements in engine technology. “We are working with DOE, other national labs, universities and industry to explore engine designs that could couple the advantages of biofuels with technologies designed to optimize their performance. Our team is examining advanced combustion technologies that could produce

improved fuel economy and lower emissions. Studies like these enable us to work in parallel to improve both engines and fuel at the same time.”

At first glance, the applied research conducted by Bunting and other fuels researchers at FEERC appears very different from that taking place in the bioenergy laboratories. The reality, however, is that these studies are just another step in the biofuels development process that spans disciplines ranging from land-use planning and agronomy to molecular biology and materials science. More important, this particular step bridges the gap between the concept of sustainable biofuels and the goal of a marketable product that could contribute to greater domestic production in the transportation fuels sector. Bunting is optimistic about the potential of biofuels to reach this ambitious goal. “I like to say we are gathering data that will be used by others to make decisions about future fuels,” he explains. “We cannot tell energy companies what to make, but we are providing solid research to help guide their decisions. I think that’s the most positive benefit of this research—working with these companies to help shape the future.” ®



A specially instrumented engine evaluates new biofuels.

A SUSTAINED EFFORT

New crops produce biofuels, but are they sustainable?

Established in 2007, ORNL's Bioenergy Science Center (BESC) could be viewed as the heir to decades of innovative environmental research at the laboratory. The first environmental studies at ORNL were conducted in the 1950s. Over the past three decades, researchers developed a comprehensive portfolio of research data from their studies of biofeedstock options and dedicated bioenergy crops. Today the center has more than 80 staff members working on diverse aspects of bioenergy, including systems biology, transportation analysis, and the impact of various bioenergy options on the environment. Their work provides a significant contribution to national and international policy debates. Among the most notable examples of these contributions is the "Billion Ton Study," a 2006 document that explored issues associated with the possibility of sustainably producing one billion tons of biomass feedstock annually in the United States.

Building on this legacy, ORNL's Center for BioEnergy Sustainability (CBES) is emerging as a valuable resource for under-

standing the challenges of sustaining the growth of biofeedstocks and the environmental considerations necessary for the production and distribution of biofuels and other bio-based products. "One of the center's primary goals is to foster communication among scientific teams at the laboratory as well as among national and international research groups who are studying many of these same issues," says CBES Director Virginia Dale. "We would like to expand their research focus to elements of sustainability along the entire supply chain."

The CBES performs work designed to complement the research at BESC, where scientists are seeking to unlock the secrets of cellulosic biofuels. CBES studies of how soils, economic factors and land use affect where energy crops can be grown dovetail nicely with BESC's development of new and improved poplar and switchgrass feedstocks. "CBES provides valuable information about available land where biomass can best be grown to enhance sustainability," Dale says. "Our researchers employ a suite of computer models to

Researchers develop a variety of new biofeedstocks in ORNL's greenhouse.



arrive at these determinations. Databases maintained at ORNL and elsewhere contribute to these models, as does the long history of involvement in feedstock development.” Robin Graham, leader of ORNL’s Renewable Energy Systems group, notes that the Environmental Sciences Division was asked by the Department of Energy in the late 1970s to identify which feedstocks would be suitable for bioenergy. Over the next three decades researchers considered a range of issues, including which species would be good bioenergy candidates, their potential for improvement, the cost of production and factors associated with harvesting and transportation to the biorefinery. “ORNL has always been the lab upon which DOE relied to determine which feedstocks are available now and which ones might be options in the future,” she says.

In recent years, CBES has collaborated with the University of Tennessee and other institutions to design large-scale experiments that examine the environmental, social and economic consequences of biomass production. The experiments enable researchers to compare plantings of traditional crops with bioenergy crops to determine the relative effects on soil, water quality and yield per acre. “When BESC has a bioenergy crop ready for field tests,” Dale says, “we have locations and experimental designs for studies that include ‘control’ groups of traditional crops, along with native and hybrid switchgrass. The studies enable us to compare the effects of growing different bioenergy crops.” Designing experiments on a large scale makes it possible for CBES researchers to incorporate ecological factors that are not practical in smaller “field plot” experiments. This analysis in turn provides the BESC with information about the sustainability of potential feedstocks.

“There are always tradeoffs,” Dale says. “We would like to find crops and management systems that are compatible with good water quality and soil conditions and that provide a desirable habitat for birds, beneficial insects and other animals. Ideally, growing and harvesting the crop would also result in low greenhouse gas

emissions, while allowing farmers to use their existing equipment. And of course, the crops must generate a profit for the farmer. We are working on analytical approaches that consider these tradeoffs.”

Graham adds that the data CBES provides on sustainability can be of use to BESC at several stages in the feedstock development process. “Some of the studies we conduct on land use and logistics provide BESC with a framework of desirable characteristics for crops that have high potential for cultivation in a particular area,” she says. “Conversely, once the plants are created, we can test them in the field and provide feedback on their potential implications for economic, environmental and social factors.”

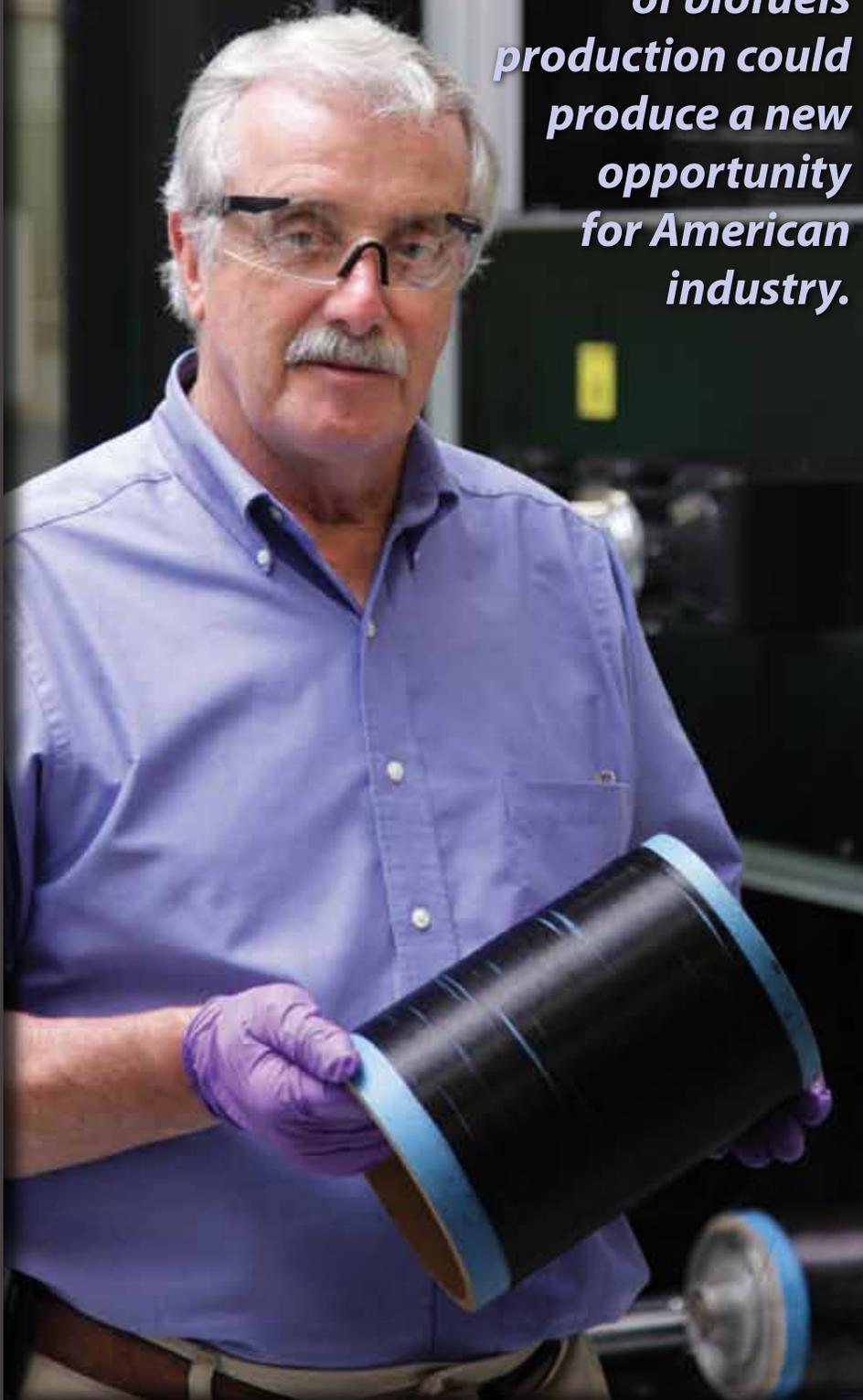
CBES has an international perspective on developing flexible approaches to cultivation of bioenergy crops. Experience has shown that crops and management practices do not migrate smoothly to every location, requiring different strategies for various regions. The optimum biofeedstock depends on a range of unique factors, including local needs for food crops, soil quality, and the crops local farmers are accustomed to growing.

“International groups are currently in the process of developing standards for feedstocks,” Dale says. “We are part of their teams, which is important because conditions for farmers in the U.S. differ greatly from those of farmers in Africa and South America. Considering the full range of approaches is critical to the fieldwork and the modeling of feedstock production.”

Both Dale and Graham agree that concerns about the sustainability of feedstocks are intensified by America’s goal of replacing a large fraction of oil imports with biofuels. Perhaps fortunately, these concerns are not unique to the United States. The international community has an increasing need for data on the sustainability of biofeedstock production, as well as on the production, use and sustainability of biofuels. Addressing this need will likely shape the next generation of environmental research at Oak Ridge National Laboratory. **R**

SOMETHING SPECIAL

A byproduct of biofuels production could produce a new opportunity for American industry.



Some projections indicate that within two decades U.S. production of fuel from biomass could exceed a billion gallons annually. If these predictions are accurate, simple arithmetic suggests that disposing of lignin, the primary byproduct of manufacturing biofuels, will present scientists with both a challenge and an opportunity. For every pound of sugar-yielding cellulose extracted from biomass, about half a pound of lignin remains. Rather than sending the waste material to landfills or burning it to heat buildings, researchers now advocate turning this waste into a variety of useful products. At a minimum, these new products could offset the cost of biofuels production. In the most optimistic scenario, creative uses for lignin could represent a transformational technology with virtually unlimited potential for American industry.

At ORNL, researchers are focused on converting lignin to carbon fiber. Materials scientist Fred Baker notes that ORNL's decade-old carbon fiber research program is driven by a simple objective: to find a way to produce carbon fiber at a low cost. The largest potential market for carbon fiber is the automotive industry. Researchers calculate that if carbon fiber could be produced and sold at a price comparable to that of the amount of steel it would replace, the weight of an average automobile could be reduced by as much as 60 percent. At present, the cost of carbon fiber is far from competitive. Suitable-quality fiber currently costs about \$15 per pound. U.S. automotive industry spokespersons suggest carbon fiber would

be substituted on a large scale if the price comes down to \$5-\$7 per pound, Baker says. "Carbon fiber is already used in some high-performance vehicles, but current costs remain prohibitive for the majority of domestic automobiles."

Baker explains that 50 percent of the cost of producing conventional carbon fiber is associated with the precursor material called polyacrylonitrile, a petroleum-based product. More than 90 percent of the 50,000 tons of carbon fiber produced annually worldwide is made from polyacrylonitrile. "That's the low-hanging fruit," he says. "If we can reduce the cost of material substantially by using lignin as a precursor, we can also reduce the cost of the finished product." In their effort to engineer a low-cost, lignin-based alternative, Baker and his colleagues examine every stage of the carbon fiber manufacturing process. They look for opportunities to save time and energy with a goal of saving money. "This is not blue-sky research," Baker emphasizes. "We have a specific purpose in mind. We are on track to produce a lignin-based carbon fiber for about \$3.50 per pound, which could be sold commercially for about \$5.50 per pound—well inside the target range." Targets notwithstanding, Baker concedes a number of engineering hurdles remain.

Baker estimates that he and his colleagues are about 60 to 70 percent of the way toward producing commercial-grade, lignin-based carbon fiber. "We know where we have fundamental issues to address," Baker says. Many of these challenges are related to the structural properties of the lignin, so his group has been working closely over the last year with ORNL's BioEnergy Science Center to implement ways of modifying these properties. Rather than employ the relatively expensive approach of chemically processing the lignin to optimize its structure for carbon-fiber production, Baker prefers to manipulate the chemistry of lignin at the source of production, in the plant. "Some researchers think the idea is far-fetched," he says, "but it's not. The process actually occurs every day in the forest products industry. The trees that

are grown today to make paper are very different from the trees that were grown 50 years ago. Today's trees have been genetically engineered to provide the best cellulose fibers for paper production. We hope to do exactly the same for lignin. Optimizing the quality of the lignin in the tree or plant would be a much more efficient process."

While producing lightweight vehicle components is the group's primary goal, Baker's team has determined that carbon fiber can be used for a range of diverse applications. Carbon fiber reinforcement has been demonstrated to reduce cracking

If carbon fiber could be produced and sold at a price comparable to that of the amount of steel it would replace in a vehicle, the weight of an average automobile could be reduced by as much as 60 percent.

in the electrodes used in steel recycling operations. The team is about 80 percent of the way toward the goal of making a lignin-based product for this application. Researchers also are investigating the fiber for use in energy storage applications, such as increasing the surface area of supercapacitor electrodes. In a supercapacitor, surface area translates directly into electrical storage capacity. Lignin-based carbon electrodes can be structured to provide thousands of square meters of surface area within just one gram of material. These components have potential applications in several industries, including the next generation of charging systems for electric vehicles.

One of the more creative potential applications for carbon fiber involves using an electric vehicle's body panels as part of an energy storage system. Structural elements that could do double duty as electrical storage devices would be immensely helpful in overcoming the size and weight of batteries—currently one of the biggest drawbacks of electric vehicles. The ability to reduce the weight and expand the power of electric vehicles simultaneously would be another transformational step in transportation technology.

One indicator of confidence in ORNL's carbon materials research comes from

the Department of Energy, which in the summer of 2010 awarded \$34.7 million to ORNL for the construction of a Carbon Fiber Technology Center. Baker says the center will not only accelerate the pace of carbon fiber research but will also fill a long-standing need for small production runs of carbon fiber made from lignin and other precursors that are needed to bridge the gap between experimentation and commercial viability. "The world's leading automakers require a minimum of one ton of carbon fiber to begin basic testing on the manufacturing of carbon fiber car parts," he says. "To manufacture and

test carbon fiber wind turbines, General Electric needs one ton for each blade, and they would rather have twice that much." The Carbon Fiber Technology Center will be able to meet research needs similar to these and will have the capacity to produce 25 tons of carbon fiber annually.

Both the new Carbon Fiber Technology Center and the range of applications to which carbon fiber technology is being applied speak volumes about the progress ORNL and the Department of Energy have made in the field of carbon materials research. The progress is even more impressive when one considers the role carbon fiber could play in increasing the commercial viability of biofuels and boosting the production of lighter-weight, fuel-efficient vehicles.

Becoming reflective, Baker looks at his research as being the beginning of something much larger. "The question regarding biorefineries has always been what to do with all the lignin when we start making vast amounts of biofuel? If we can learn how to turn a waste material into useful products that reduce the cost of biofuel, reduce our dependency on oil imports and spawn a new sustainable sector of American industry, then we are indeed talking about something special." 

Martin KELLER

, ORNL's Associate Laboratory Director for Biological and Environmental Sciences, has responsibility for two research divisions (Biosciences and Environmental Sciences) and four research centers (the BioEnergy Science Center, the Center for BioEnergy Sustainability, the Center for Molecular Biophysics and the Center for Structural Molecular Biology). Keller came to his current position from his previous role as Director of the lab's Biosciences Division.

We asked Keller about his organization's role in addressing some of the Department of Energy's key research challenges.

You spent a number of years working in the private sector. How does that experience compare with working at a national lab?

I spent ten years working at a biology company that started with 6 or 7 people and grew to about 400. The major difference between that company and a national laboratory is that things move faster in an organization that small. On the other hand, small companies are often preoccupied with intellectual property, so it's hard to publish an abstract or make a presentation at a meeting without having to deal with intellectual property concerns. These concerns can slow down both communication and the scientific process. In most respects, research in the national laboratories is much like that in private companies, except the "R" in "R&D" is bigger. We do more research and less development. That's a good thing. I'm a supporter of targeted fundamental research. We need to understand fundamental science to enable the development of new processes.

What initially attracted you to ORNL's biosciences program?

After ten years in the biotechnology industry, I thought that it was time to move on. I had a couple of opportunities to go back to academics or to other biotech companies, but I decided to come to ORNL because a national laboratory is the only place where researchers can work across the range of disciplines necessary to rapidly advance science. ORNL can bring together specialists in sustainability, biochemistry, materials research, computer modeling and other areas to address issues. That breadth of capabilities is not present in most other organizations.

Your organization is involved in interdisciplinary research across the laboratory. What benefits does this approach to R&D provide?

Let's take carbon fiber as an example. Carbon fiber can be produced from lignin, a byproduct of biofuel production. Carbon fiber can be used to create lightweight, high-strength components like body panels for cars, so there's a lot of interest in finding a way to produce high-quality, low-cost carbon fiber derived from lignin. If we kept each research discipline related to the production and use of carbon fiber in its own little stovepipe, we would miss the opportunities for synergies among these disciplines that might completely change our business model. We have scientists who know how to create carbon fiber from lignin, but they would like the lignin to have different properties that would result in better carbon fiber. We also have plant biologists who can manipulate the genetics of plants to produce very different lignin structures, but they are unfamiliar with what is required to produce high-quality carbon fiber. Neither group working individually can solve the problem; however, when we bring these two groups together, we can advance the technology.

Climate research has been assigned a high priority at ORNL. What is your directorate doing to support this mission?

Climate research is another example of a field where interdisciplinary research is increasingly important. Scientists specializing in genomics, proteomics and molecular biology are working with specialists in global climate simulation using the laboratory's Jaguar supercomputer. Many climate-related problems cannot be addressed through a single discipline. For example, we are planning an experiment in which plots of arctic soil that were previously covered with snow and ice will be warmed to determine how the carbon trapped in the soil will be released to the atmosphere. Will it be released as CO₂? Will microbes in the soil degrade carbon to CO₂ or methane? We don't know, but the data resulting from the study could have a tremendous impact on climate models.

DOE has a lot riding on the BioEnergy Science Center. What do you see as the primary challenge for the center?

I always say that in a large research project, particularly in interdisciplinary research, the biggest challenge is communication. If we bring a molecular biologist together with a computer scientist, we find out that they often don't speak the same scientific language. They have to invest the time to learn enough about each other's specialty to be able to communicate and to cooperate to reach common goals. In BESC we have made tremendous progress in communication to help our 320 staff members come up with a common language that enables them to work together effectively.

Now that we have overcome most of our communication obstacles, our biggest challenge is determining which of several very promising lines of bioenergy research will have the greatest impact in helping to create a biofuels industry. We have made astonishing progress in a number of areas, but we do not have the resources required to concentrate on all of them. The decision is similar to having a table full of delicious food, but being able to choose only two or three items.

What changes might the average consumer see in the use and availability of biofuels over the next ten years?

That's a tough question. I would say we absolutely will have the technology to establish a sustainable biofuels industry in ten years. There is no longer any doubt; it will happen. The more precise question is whether as a nation we want to do it. If we choose to have a viable biofuels industry ten years from now, there are a number of policy issues that must be addressed quickly. Which biomass crops will we use? Where will we plant them? Are farmers ready to make the transition to biomass? Where will the bioprocessing plants be sited?

In the next ten years, we will be capable of producing several blendable biofuels that can go into our standard fuel system. We will also have the option of planting a variety of different biomass crops, as well as producing a range of products, like carbon fiber, from bioprocessing byproducts. Will all this happen in ten years? It could. If we keep on the path and retain our commitment to biofuels as an alternative to imported oil, then this is the future we are moving toward. 



ORNL Researchers Win Nine R&D 100 Awards

Researchers at Oak Ridge National Laboratory were honored with nine awards in *R&D Magazine's* annual selection of the year's 100 most technologically significant new products of 2010. Sometimes referred to as the "Academy Awards of Science," this year's nine winners bring to 156 the total number of R&D 100 awards won by ORNL scientists.

Telemedical Retinal Image Analysis and Diagnosis (TRIAD).

Submitted by ORNL, Automated Medical Diagnostics and the University of Tennessee Health Science Center. ORNL team members: Kenneth Tobin, Thomas Karnowski, Luca Giancardo, Deniz Aykac and Priya Govindasamy. UTHSC team members: Edward Chaum and Yaqin Lee

The TRIAD technology is a Web-based telemedical diagnostic system designed to conduct automated eye screenings of large patient populations for blinding diseases, such as diabetic retinopathy, in a primary health care setting. The real-time, low-cost screening provided by TRIAD assists primary care providers in offering a more efficient and economical retina screening service to prevent blindness in diabetic patients. The diagnostic tool will enable more people to undergo screening, especially the indigent and those in areas that are medically underserved. Research funding was provided by ORNL's Laboratory Directed Research and Development (LDRD) program, the Plough Foundation, Research to Prevent Blindness, the U.S. Health Resource Services Administration and the National Institutes of Health - National Eye Institute.

Liquid Microjunction Surface Sampling Probe for Mass Spectrometry.

Submitted by ORNL and NextGen Services. ORNL team members: Gary Van Berkel and Vilmos Kertesz

The ambient surface sampling system for mass spectrometry uses a sampling probe for quick, efficient liquid extraction of analytes directly from surfaces. The system's ability to analyze materials outside a vacuum and under real-world conditions demonstrates a significant improvement over existing technologies, limited to surface sampling within a vacuum. The product's simplicity, speed and cost effectiveness make possible a range of uses within the biological sciences, including applications in pharmaceutical research and drug discovery. Research was funded by ORNL's LDRD program, the Department of Energy's (DOE) Office of Science, a CRADA with MDS Sciex, UT-Battelle's Privately Funded Technology Transfer Program and ORNL royalty maturation funding.

Sulfur-Carbon Nanocomposite Cathode Material and Additives for Lithium-Sulfur Batteries.

Submitted by ORNL. Team members: Chengdu Liang and Nancy Dudney

The technology offers a more functional sulfur-carbon nanocomposite cathode and halide additives to the electrolyte to solve problems inherent in existing lithium-ion battery technology. Researchers hope the lithium-sulfur battery system can improve the energy density of current technologies by a factor of five. By enabling a more reliable, safer and longer lasting battery system, the invention has the potential to aid in the harnessing, storage and use of electricity from renewable energy sources. The project was funded by ORNL seed money and the DOE's Vehicle Technology program.

Ultrasensitive Nanomechanical Transducers Based on Nonlinear Resonance.

Submitted by ORNL. Team members: Nickolay Lavrik and Panos Datskos

Based on nonlinear nanomechanical resonators, the technology enables sensitive linear detection of force or mass that can be used in a number of important applications, including chemical and biological detection, inertial navigation and thermal imaging. The technology can identify the presence of extremely low levels (femtogram quantities) of chemicals in a gas or liquid with a sensitivity 1,000 times greater than that of comparable mass-sensitive transducers on the market. The new method used in the nonlinear resonator transducers can provide real-time monitoring in a cost-effective manner and can lower detection thresholds in both gas and liquid environments, without increasing the cost and complexity of the tool. Research funding was provided through ORNL's LDRD program.

Strontium Iodide Scintillator for Gamma Ray Spectroscopy.

Submitted by Lawrence Livermore National Laboratory and developed in conjunction with ORNL, Fisk University, Radiation Monitoring Devices Inc. and the Department of Homeland Security's Domestic Nuclear Detection Office. ORNL team members: Lynn Boatner, Joanne Ramey and James Kolopus

The technology allows for the precise detection of illicit sources of uranium, plutonium and other radioactive materials, which can play a critical role in identifying nuclear and radiological threats. Europium-doped strontium iodide enables the highest-resolution gamma-ray spectroscopy for a scintillator detector to identify radionuclides. The technology's superior scintillator energy resolution and cost-effective production will prove invaluable for homeland security applications. Research was funded through the DHS Domestic Nuclear Detection Office.

Mode-Synthesizing Atomic Force Microscope (MSAFM).

Submitted by ORNL. Team members: Ali Passian, Thomas Thundat and Laurene Tetard

MSAFM is a novel measurement system for noninvasive, high-resolution surface and subsurface characterization and analysis of materials at the nanoscale. The technology can obtain a wealth of material information from both the surface and the subsurface domain, opening unlimited opportunities in nanoscience in a variety of endeavors, including human health, environmental studies, toxicology, nanofabrication, cell mechanics and energy research. Research was sponsored by the DOE's BioEnergy Science Center at ORNL.

High-Performance, High-Tc Superconducting Wires Enabled via Self-assembly of Non-superconducting Columnar Defects.

Submitted by ORNL, SuperPower Inc., the University of Houston, and the University of Tennessee. ORNL team members: Amit Goyal, Sung-hun Wee, Eliot Specht, Yanfei Gao, Karren More, Claudia Cantoni, Keith Leonard, Malcolm Stocks, Tolga Aytug, Mariappan Paranthaman, David Christen, Jim Thompson and Dominic Lee

The technology is a three-dimensional self-assembly process for the fabrication of ultrahigh-performance superconducting wires. The method is designed to create non-superconducting nanoscale columnar defects with nanoscale spacing within high-temperature superconducting wires. The desirable defects can improve the performance of high-temperature superconductors by enabling large currents to flow through the materials in the presence of high applied magnetic fields. The need for high-temperature superconductors in the electric power, medical, transportation, industrial and military sectors demonstrates the product's commercial viability. The research was funded through the DOE's Office of Electricity Delivery and Energy Reliability and ORNL's LDRD program.

Flexible, Large-area, Single-Crystal-like, Semiconductor Substrates.

Submitted by ORNL and TexMat. ORNL researcher: Amit Goyal

The technology results in a large-area, flexible substrate with a single-crystal-like semiconductor surface. The process starts with a textured metal or alloy substrate upon which various multilayers are grown heteroepitaxially, leading to a semiconductor surface. Further epitaxial growth of device layers on such substrates is used to fabricate devices for electronic applications such as photovoltaics, displays, ferroelectrics, solid-state lighting, and assorted sensors. Such flexible substrates potentially can be made in sizes that are orders of magnitude greater than is currently possible with standard rigid semiconductor wafers. Research at ORNL was supported by a work-for-others project.

Ztherm Modulated Thermal Analysis.

Submitted by ORNL and Asylum Research Company. ORNL team members: Maxim Nikiforov, Sergei Kalinin and Stephen Jesse

The team developed a tool for failure analysis of devices such as electrical conductors or semiconductors in flexible electronic devices and polymer photovoltaic devices, in which polymers play a key role. Ztherm Modulated Thermal Analysis offers highly localized heating with sensitivity to sub-zeptoliter material property change, with significant improvements over other commercial systems. Ztherm is an effective method for characterizing the mechanical properties of polymers as a function of temperature with the highest spatial resolution available today. A portion of this research was conducted at ORNL's Center for Nanophase Materials Sciences, sponsored by DOE's Office of Science. 



...and the WINNERS

Accomplishments of Distinction
at Oak Ridge National Laboratory are...

Michael K. Miller has been named a **UT-Battelle Corporate Fellow**. The honor is UT-Battelle's highest level of recognition for career achievements in science and technology, performance and leadership.

Laboratory Director **Thom Mason** has been appointed **Corporate Chair** of the local chapter of the **East Tennessee Branch of the Juvenile Diabetes Research Foundation**.

Michelle Buchanan, Associate Laboratory Director for Physical Sciences, has been named a **Fellow** of the **American Chemical Society**.

Martin Peng has been awarded the **2010 FPA Leadership Award** by the **Fusion Power Associates** board of directors, for his outstanding leadership qualities in accelerating the development of fusion as an energy source.

Theodore Besmann has been named a **Fellow** of the **American Nuclear Society**.

Brian Wirth has been appointed to fill the ninth **University of Tennessee–Oak Ridge National Laboratory Governor's Chair**.

Albdolreza Zaltash has been named a **Fellow** of the **American Society of Mechanical Engineers**.

Gary L. Baker has received the **George W. Thorn Award** from the **University of Buffalo (SUNY)**.

Gonzalo Alvarez and **Viviane Schwartz** have been named to the **40 under 40 in Science, Technology, Engineering and Mathematics** list by **Hispanic Engineer & Information Technology** magazine.

Nina Balke has received the **Alexander Von Humboldt Research Fellowship** from the **Alexander von Humboldt Foundation**.

Oak Ridge National Laboratory, in collaboration with several other institutions, received the **Secretary of Energy's Excellence in Acquisition Award** from the **U.S. Department of Energy**, for the design and construction of TEAM, the world's most powerful electron microscope. The project was led by **Lawrence Berkeley National Laboratory**. ®

Michael Miller

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