

Breakthroughs

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FALL 2006

CREATIVE ENERGY

PNNL researchers
are generating
real-world
solutions to a
global problem



Pacific Northwest National Laboratory

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Converting energy resources... and ourselves

Every time I put together an issue of Breakthroughs, I learn a lot. So far, though, this is the first issue that has motivated me to change my own behavior and thinking.

Yes, like most people I shake my head every month when I get my electric bill; I lamely kick my tire as the numbers on the gas pump roll faster than I can count. Energy is a big deal on a personal level. But reading through the special section articles, I was jolted by the reality of what is happening to our country. And sadly, it's within our power to fix the problem.

The good news is that I work at a place that focuses every day on the growing energy problem. The special section features work on many fronts: grid, nuclear, coal and hydrocarbon conversion. The bad news is that it will take time and money to develop solutions into working technologies and processes. But have faith. These are very talented people.

While I cannot match the scientific creativity of PNNL's staff, I can take my new-found knowledge and apply it. I've already installed my first compact fluorescent light (CFL). And the next time I buy coffee, I'll walk into the store rather than idle in the drive-through—less gas, less pollution. We all can contribute something. — LT



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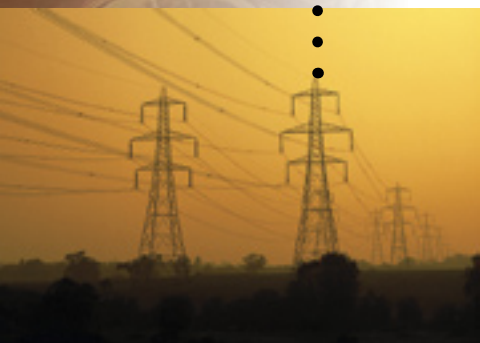
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Coastal ecosystem expert on board with Marine Research Operations

Andrea Copping, a biological oceanographer, has come from the deep blue sea to join Pacific Northwest National Laboratory's Marine Research Operations in Sequim, Washington. Copping, a senior program manager for marine and coastal waters, is working with federal, state and local agencies on strategies and issues relating to the cleanup, restoration and protection of Puget Sound.

Before coming to PNNL, Copping was the associate director of the Washington Sea Grant Program at the University of Washington. She will maintain her university ties as an associate professor in the UW School of

Marine Affairs. With a doctoral degree in biological oceanography, Copping brings more than two decades of marine research and institutional knowledge to PNNL, including experience in directing the Pacific Northwest Regional Marine Research program, environmental consulting and serving as president for the Pacific Estuarine Research Society.

Marine Research Operations is the Department of Energy's only marine research laboratory. Using state-of-the-art equipment and facilities, the laboratory is advancing the understanding of marine environments to solve problems and protect and

manage valuable marine resources.

Principal capabilities at the facility include marine and freshwater ecotoxicology, organic chemistry, environmental forensics, coastal and wetland restoration, fisheries studies, research in remediation technologies and biotechnology and fate-and-transport modeling in ocean and near-shore regions. ●



Andrea Copping

PNNL Laboratory Fellow appointed to Mars exploration committee



Jim Fredrickson

Committee on the Astrobiology Strategy for the Exploration of Mars. The committee, whose assignment ends in September 2007, is undertaking a study that defines a scientific strategy for the search for life on Mars. Funded by NASA, the study will encompass

Laboratory Fellow Jim Fredrickson, Pacific Northwest National Laboratory, accepted an appointment on the National Research Council's

both biological and environmental perspectives relevant to the search for life, as well as build path-forward strategies including scientific goals, objectives, investigations and priorities.

This integrated team of managers, scientists and engineers will respond to the scientific and resource challenges associated with deep space exploration of the Red Planet. By the end of the first decade of the Mars Exploration Program, scientists may know where and how to look for the elusive clues associated with a possible fossilized biological record of life.

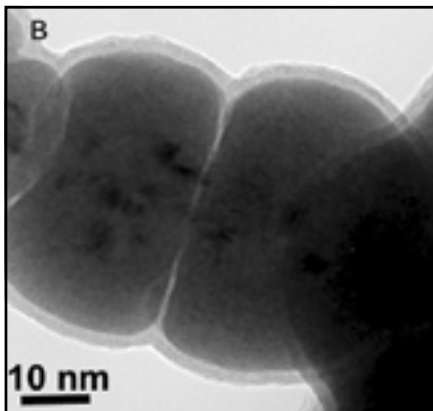
Fredrickson was invited to join after the committee learned of his vast experience in microbiology and subsurface microbiology. The committee felt his expertise in this area would bring

a new perspective to the group's diverse background. Specifically, Fredrickson's role will be to provide insight into various aspects regarding the potential for past and present microbial life on Mars, including current environments that may support life and the types of metabolic signatures indicative of past-life activity.

At PNNL, Fredrickson is a chief scientist in the Biological Sciences Division. He leads a range of research projects, including the *Shewanella* Federation, part of the Genomics: Genomes to Life program managed by the Department of Energy's Office of Biological and Environmental Research. He also participates in the Grand Challenge in Biogeochemistry. ●

Sometimes smaller is better

A research team from the Pacific Northwest National Laboratory, Oregon Health and Science University, University of Minnesota and the University of Idaho is studying the ability of nanoscale iron



This high-resolution transmission electron microscopy image of a metallic iron nanoparticle shows the nature of its “protecting” shell. The chemistry of the shell appears to be crucial to the nanoparticle’s ability to react with carbon tetrachloride to produce harmless byproducts.

particles to reduce carbon tetrachloride, a common groundwater contaminant.

In the past, carbon tetrachloride was a common component in refrigerants, industrial degreasers and pesticides. This chemical is now an environmental contaminant, and according to the U.S. Environmental Protection Agency, carbon tetrachloride can cause liver, kidney and central nervous system damage.

One remediation method for contaminated groundwater uses microsized iron particles that react on contact with carbon tetrachloride. However, the reaction often produces chloroform, another environmentally undesirable chemical.

The research team’s studies indicate that one type of nanosized iron particle can be more effective in reducing carbon tetrachloride in water than the microsized particles while also minimizing the production of chloroform.

“The use of nanosized particles of iron for cleaning up contaminants

in groundwater, soil and sediments is an exciting new technology that contributes to a general enthusiasm about nanotechnology,” said Don Baer, the project’s principal investigator from PNNL.

The researchers examined two iron nanoparticles, one produced by the hydrogen reduction of an iron oxide (FeH₂) and the other produced by a solution synthesis (FeBH) method. The FeH₂ particles had a shell made of iron oxide, and the FeBH had a shell that included boron oxide as well as iron oxide. The research study involved both the characterization of the particles and examination of their reactivity. The team determined that FeH₂ produced lower quantities of chloroform in comparison to FeBH or micron-sized particles of iron.

This study suggests that nanosized iron particles with the right chemistry may be the better ingredient for new technologies to clean up carbon tetrachloride in contaminated groundwater sites around the country. ●

Structural safety gets boost from new technology

An acoustic inspection technology developed at Pacific Northwest National Laboratory may help users in the oil, gas and other industries decide if a metal structure can withstand normal operation. Using a newly developed ultrasonic measurement technology, PNNL researcher Paul Panetta and his team can rapidly locate and characterize suspected damage associated with strained metal, which current technologies cannot do.

“The immediate beneficiaries of the technology are oil and gas pipeline operators because our prototype is specifically configured for characterizing damage to pipelines from landslides, earth movement and dents,” Panetta said. “Its distinctive capabilities can enhance existing inspection technologies to help avoid pipeline failures—sometimes catastrophic ones.”

A bend, bulge or dent in a pipeline or other metal structure is sometimes obvious, but the extent of the damage is not. This measurement technology uses ultrasound to determine the material properties of metal to determine the extent of damage caused by natural disasters, accidental run-ins with heavy equipment or normal wear and tear.

“Pipes are typically assessed with in-line inspection tools, commonly referred to as ‘pigs’ in the oil and gas industry,” Panetta said. “Pigs typically only show wall thinning or detect the presence of dents, which may not indicate if the damage is detrimental.”

The technology can be used for assessing the integrity of pipelines, bridges, railroad tracks and cars, steel girders, airplane landing gear or other metal structures. It was originally

developed for the Department of Energy for use in natural gas pipelines and is currently available for licensing. ●



A prototype manual scanner of the ultrasound pipe crawler is tested on a metal pipe by researchers from the Pacific Northwest National Laboratory. This technology is designed to help users in the oil, gas and other industries determine the integrity of metal structures.

ScalaBLAST solves problems in record time

“Remember that time is money.”

– BENJAMIN FRANKLIN

Scientists are dedicated to making discoveries that influence our world, but making these discoveries takes time. It took Albert Einstein 16 years to express his general theory of relativity. Benjamin Franklin was first introduced to electricity experiments on a trip to Boston in 1746, but his famous lightning rod experiment didn't occur until six years later—and he knocked himself unconscious more than once in the process. Of course, Al and Ben didn't have the luxury of computing technologies and tools either.

Today we have ScalaBLAST, a computational tool developed at the Pacific Northwest National Laboratory based on BLAST, a conventional sequence analysis tool developed by the National Center for Biotechnology Information (NCBI). ScalaBLAST is dramatically speeding up our understanding of the

machinery of life—bringing us one step closer to curing diseases, finding safer ways to clean up the environment and protecting the country against biological threats. ScalaBLAST uses innovative high-performance computing software such as the Global Arrays Toolkit to perform sophisticated sequence alignment of proteins. Now, large-scale problems—such as the simultaneous analysis of hundreds of organisms—can be solved in hours rather than years.

Recently, PNNL scientists completed a large-scale ScalaBLAST analysis in conjunction with the Joint Genome Institute at Lawrence Berkeley National Laboratory, solving a significant “data avalanche” problem for JGI. In just 18.5 hours, 1.6 million proteins were BLASTed against NCBI's nonredundant protein database using 1500 processors, producing 75 gigabytes of analysis results—a job that would have taken just over 3 years on a single machine.



ScalaBLAST gives a sizeable performance boost over BLAST, a conventional sequence analysis tool.

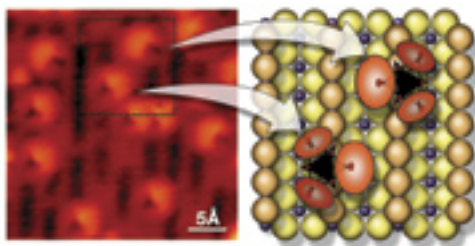
Hold onto your seats—PNNL scientists are BLASTing us into an exciting future of scientific discovery through this and other innovations extracted from the Department of Energy Office of Advanced Scientific Computing Research Data Intensive Computing for Complex Biological Systems project. But unlike Benjamin Franklin, we won't have to knock ourselves unconscious to ride along. ●

Uniform nano-clusters signal improved catalysts

A new model system of nano-structures has been synthesized and could lead to control of chemical transformations critical for enhancing the nation's energy future.

This new nanostructure model system, developed by researchers at the Pacific Northwest National Laboratory, the University of Texas-Austin (UT) and Washington State University, offers insights into the structure and reaction mechanism of metal oxides. Metal oxides are important catalysts for producing fuels for transportation and value-added chemicals.

In the new model system, nano-clusters composed of cyclic tungsten trioxide line up molecule-by-molecule on a titanium dioxide platform. One tungsten atom from each cluster is raised slightly, holding forth the potential to execute catalytic reactions—a striking



A scanning tunneling microscope image (left) shows nano-clusters deposited on a titanium dioxide platform with consistent orientation of the atoms (right). The dark triangle indicates the center of the tungsten trioxide molecular ring on the platform; the brighter side depicts the raised atom.

difference from commercial catalysts. Commercial catalysts vary in size and chemical composition, making it difficult to understand or predict the reactions taking place at the molecular level. In the new model, all the nano-clusters are the same size, evenly dispersed, and oriented in one of two directions on the titanium oxide crystal

layer. This unique, uniform feature may enable scientists to predict with increased accuracy and control the reactions that will occur, thereby enhancing the effectiveness of catalytic reactions.

The researchers employed specialized equipment at the Environmental Molecular Sciences Laboratory, a DOE user facility on the PNNL campus, to prepare and characterize the platform as well as the clusters. Using a unique approach that changed the tungsten oxide directly from a solid to a gas, the researchers successfully stabilized the molecular rings—or “trimers”—of tungsten on the titanium platform.

The new nanostructure model system was developed as part of the Early Transition Metals as Catalysts project at PNNL, supported by the DOE Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division. ●

Award-winning technologies a potential goldmine for medical, manufacturing fields

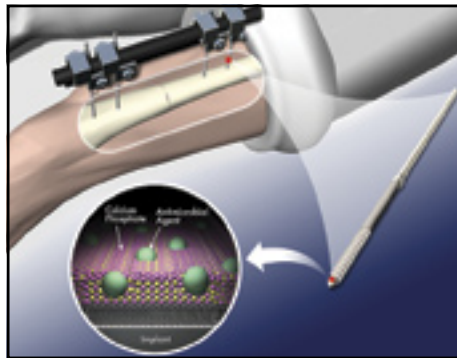
An improved cancer treatment and a new way to manufacture titanium parts are among the Pacific Northwest National Laboratory innovations that received international acclaim this year from *R&D Magazine*. Known as the “Oscars of Invention,” the R&D 100 awards honor the top 100 scientific and technical products and advancements worldwide each year.

In total, PNNL has won 71 R&D 100 awards since it first began submitting entries in 1969. The Laboratory and its partners received this year’s awards for five technologies.

Cesium-131 Brachytherapy Seed. This tiny seed, used to treat prostate and other cancers, delivers a highly targeted therapeutic dose of radiation to tumors quickly and with potentially fewer side effects than other treatment options. PNNL shared this award with IsoRay Medical, Inc., of Richland, Washington, which developed the technology with assistance from PNNL. A public company, IsoRay Medical is manufacturing the seeds and distributing them to hospitals and other medical centers nationwide.



Radiation-emitting “seeds” are being used to treat hundreds of prostate cancer patients nationwide with cesium-131, which delivers a more aggressive dose and leaves the body much faster than other isotopes, dramatically reducing unnecessary radiation exposure to nearby healthy tissue.



Applying calcium-phosphate coatings with the SIM process allows the body to accept metal implants as bone material.

SIM. This surface-induced mineralization technique allows drug-enhanced calcium-phosphate coatings to be applied to orthopedic implants and medical devices, enhancing bone-bonding and reducing bacterial growth. The technology has been licensed to Bacterin of Belgrade, Montana. When fully commercialized, the product is expected to help the body accept foreign objects like knee implants or catheters, while also inhibiting post-surgical infection. Last year, *Fortune* magazine featured the technology and Bacterin in its 25 Breakout Companies list of entrepreneurial firms.

e-RESS. This technology uses supercritical fluids and electric fields to deposit nanoparticle-size coatings onto the surfaces of medical devices such as cardiovascular stents. Therapeutic agents may also be encapsulated in the coatings, allowing for more consistent drug delivery and reducing the need for replacement surgeries caused by the buildup of tissue. PNNL shares this award with Micell Technologies of Raleigh, North Carolina, which licensed the technology this year for use with medical devices.

MilliWave Thermal Analyzer.

This patent-pending instrument uses millimeter-wave electromagnetic radiation to measure the temperature, amount of energy emitted, and physical changes of materials, processes and systems in real time. PNNL shares this award with the Massachusetts Institute of Technology in Cambridge, Massachusetts, and the Savannah River National Laboratory in Aiken, South Carolina.

Ti MIM. This technique for titanium metal injection molding that enables production of high-quality titanium metal parts for biomedical, aviation and automotive industries at lower cost, higher production rates and better quality than existing production processes. The Ti MIM process was licensed to a Fortune 500 chemical company this year. ●



Ti MIM is a proprietary binder for injection-molded titanium without impurities. For manufacturers, this means faster, lower-cost production of high-strength parts for the biomedical, aviation and automotive industries.



PNNL physicist wins presidential science award



Yanwen Zhang

In July 2006, Pacific Northwest National Laboratory's Yanwen Zhang, a materials physicist, received the Presidential Early Career Award for Scientists and Engineers. This

is the highest honor bestowed by the United States government on outstanding scientists and engineers beginning their independent career. Zhang was also presented with the Department of Energy Office of Science Early Career Scientists and Engineers award. Both awards recognize her extensive research in materials physics—most notably in ion-beam technologies.

Over a decade ago, the National Science and Technology Council created this award program to honor and support the extraordinary achievements of young professionals within the science and technology fields. Zhang was nominated by PNNL and DOE for this award, which also entails a five-year funding research commitment on behalf of DOE.

Zhang holds two doctoral degrees—one in engineering physics from Lund University in Sweden and another in materials science from Beijing Normal University in China. Currently working in the DOE Environmental Molecular Sciences Laboratory in Richland, Washington, her research focuses on the interaction of energetic ions with solid materials. Her original and innovative method for measuring the energy

loss of particles as they pass through materials solved the historical problem of inaccurate and inefficient measurements. Zhang's successfully implemented time-of-flight spectroscopy process was a significant scientific breakthrough. Her discoveries have potential impact in nuclear power, national security, nuclear waste management and energy-efficient electronics.

With more than 100 publications and several ongoing research collaborations, Zhang is widely recognized for her significant contributions to the scientific community. She also is active in several professional societies, has received other science and academic awards and is involved in educational and community service activities. ●



Technology improves food processing quality

Researchers at Pacific Northwest National Laboratory have developed an ultrasonic technology that could tell food manufacturers if foreign objects have fallen into their product long before it reaches the consumer.

The technology uses sound waves and optical capabilities to detect foreign objects in processing streams. PNNL's patented inspection method can detect cartilage, metal, plastic or anything else that should not be in the product.

Inspection methods, such as x-ray, can be costly and slow and require added safety precautions and complex operator training. The PNNL method offers the option of automation. Ultrasonic technology alleviates much of the added difficulty currently incurred

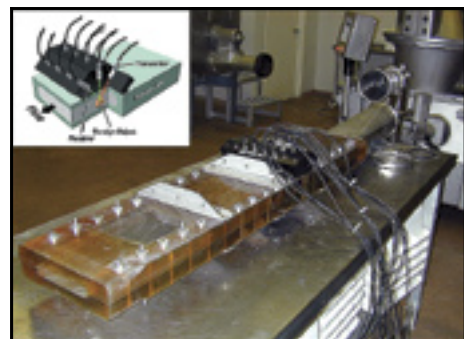
by manufacturers when inspecting processed food products manually.

“Our method is the only one we’re aware of that uses both acoustics and optics,” said Aaron Diaz, PNNL staff scientist. “Because it can be automated, it’s inherently safer and more effective than inspecting certain types of process streams manually.”

Acoustics, combined with light transmitted through the product, adds to the data extracted from the stream, making results more accurate. The two methods may be used separately, depending on the properties of the product being inspected.

This technology could bring the inspection quality of processed food to a whole new level. “It’s a useful technology that could positively impact

manufacturing in many areas,” Diaz said. More information about the technology is available at <http://availabletechnologies.pnl.gov>. ●



This prototype shows multiple acoustic and optical sensors configured along a process stream to detect foreign objects. The technology can be used to detect metal, plastic or cartilage in products such as ice cream or baby food.

CREATIVE ENERGY

PNNL researchers are generating real-world solutions to a global problem



▲ ESTD Director Mike Davis

Meeting supply and demand challenges head-on

Mike Davis joined Pacific Northwest National Laboratory as director of the Energy Science and Technology directorate in January 2005, bringing to the Laboratory 30 years' experience spanning public and private sectors. Mike oversees PNNL's energy research totaling \$93 million, which includes research and development for clean and efficient "energy supply" as well as technologies for reducing "energy demand" and increasing efficiency. These activities range from development of new materials for solid oxide fuel cells, hydrogen storage, next-generation lighting and abatement of auto emissions to technology advancements targeted at energy-smart buildings, an efficient, secure power grid and near-zero emission electricity from coal. Under Mike's leadership, PNNL is building on its extensive demand-side energy research portfolio with an expanded reach into the supply side of the energy equation. Here, Mike discusses one of these new efforts and his vision for how PNNL's expertise will help move our nation toward energy independence and a better environment and economy.

There are many schools of thought regarding the path forward to address today's energy challenges. What is your overarching philosophy?

There's an ancient Native American proverb that reads "*Treat the earth well: it was not given to you by your parents, it was loaned to you by your children. We do not inherit the Earth from our Ancestors, we borrow it from our Children.*" Our quality of life depends on energy—how we produce it, how we use it. Historically, economic drivers tended to trump environmental concerns. Our challenge today, however, is how to meet growing energy demands with domestic resources in a manner that's efficient and economical yet compatible with our environment.


How do you characterize today's energy challenge?

It's one of the biggest challenges facing our nation today. Demand for energy has doubled in the last 50 years and is projected to increase through 2025. Approximately 85 percent of that demand both domestically and globally is met through use of hydrocarbons, such as crude oil, natural gas and coal. Domestic oil production, however, has been on the decline since 1970, resulting in increased reliance on oil imports during a time of decreased global security. We're seeing the resulting hit at the pump. A barrel of oil was priced at approximately \$25 just three years ago compared to the \$60-\$70 range we're experiencing today—a 260 percent jump. The wealth transfer to foreign countries is staggering. Every \$5 increase we pay on a barrel of oil represents \$100 million moving from other areas in our economy to pay for the same amount of oil, 60 percent of which goes directly out of our country. This is a wealth transfer offshore of \$219 billion per year. No economy can sustain this level of wealth transfer. And just imagine what we could do with these billions if they were inserted back into our economy.

In addition to the economic and security concerns, the environmental impacts are real. Without technology advancements and commercial processes, we'll put more carbon, a byproduct of using hydrocarbon-based energy resources, in the air in the next 50 years than we have in the last 200. That prospect, along with our unsustainable wealth transfer, should motivate our best efforts for solutions.

Where does the solution lie?

Energy sources such as renewables, hydrogen and nuclear power will play an increasingly prominent role in our nation's energy supply, but these resources are 25 years away from scaling up to meet global energy demand. Today, we need a clean, secure "energy bridge" to help transition the global economy to a future renewable, nuclear and hydrogen energy base. At PNNL, we're assessing what we believe to



be a promising contender for this bridge—domestic hydrocarbons used in air emissions- and water-neutral manner.

While the world may be approaching peak production of readily accessible, high-quality hydrocarbons such as sweet/light crude oil, the United States has substantial reserves of lower-quality hydrocarbons such as coals, oil shales and biomass. Our challenge lies primarily in cleanly and economically converting these resources into liquid transportation fuels to reduce our reliance on oil imports. The conversion concept focuses on gasifying the coal versus burning it and capturing and sequestering the CO₂ normally released in the process. The resulting end product would be a type of liquid fuel that could be sent to conventional refineries for conversion into finished chemicals or fuels. The U.S. is home to 25 percent of the world's coal supplies, yet we import millions of gallons of oil per day. Finding a way to use our coal resources cleanly and economically to meet our growing demand for transportation fuels holds great promise for reducing our dependence on imported oil.

What does PNNL bring to the table?

PNNL has been actively involved in assessing the business realities surrounding expanded use of our coal and biomass resources, working closely with state and federal governments. From a technical perspective, the science base at PNNL is in direct alignment with capabilities and expertise required to address the challenges I see throughout this 50-year bridge. In addition to our leadership role in carbon capture and sequestration research, our expertise in gasification, separations, chemistry and catalysis positions the Laboratory central to the solution. We also are expanding linkages with the private sector. These partnerships are critical to ensuring that the output of the science base provides solutions that work within existing infrastructures in real-world environments and markets.

What's your vision for the future?

I envision broad, clean and efficient use of our domestic resources, which will result in relief from our overdependence on imported oil and serve as a secure bridge to a viable, clean and independent energy future. If we can accomplish this, we may have answered the call of leaving the world a better place for generations to come.

PNNL positioned to meet nation's energy challenges

Innovative science and technological advances will play a key role in solving the energy challenges facing the United States, and PNNL stands ready to help.

"I don't think there's a more important problem in the world right now, both near- and long-term, than energy," said Jud Virden, director of Energy Programs Business Development. Virden leads the charge to align the Laboratory's science and technology contributions with the nation's energy mission and to execute related business opportunities.

PNNL is addressing the energy challenge with research across the entire energy spectrum—from cleaner and more efficient uses of fossil fuels to next-generation nuclear technologies, to a more reliable electricity grid to energy efficient demand-side technologies.

Hydrocarbon Conversion

A major focus of PNNL's energy research is exploring "air- and water-neutral" conversion of domestic hydrocarbons such as coal to liquid transportation fuels, specifically finding ways to design plants that capture and safely store emissions and use as little water as possible (see related story, page 11).

PNNL's catalysis expertise, as well as biofungal capability, also will be applied in advanced research to convert biomass, another hydrocarbon, to transportation fuel and chemicals at the Bioproducts, Sciences, and Engineering Laboratory (BSEL) being built in Richland, Washington. BSEL is a multi-user facility established jointly by PNNL and Washington State University.

Power Grid Reliability

The Laboratory is heavily involved in research activities to enable enhanced grid reliability and productivity, including building capabilities for wide-area monitoring and real-time analysis of grid operations.

In 2006, PNNL established the Electricity Infrastructure Operations Center, a user-based facility dedicated to energy and hydropower research and operations training. One focus of the facility is to use advanced software to process data in real time to enable a better handle on the current status of the grid as well as predict how the grid will behave in the near future (see related stories, pages 12 and 13).

Expansion of Nuclear Power

The interest in nuclear power is on the rise as energy demands continue to grow. PNNL, which has world-class

... continued; see "**Energy Challenges**" (page 10)

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PNNL researchers are generating real-world solutions to a global problem

Energy Challenges (continued from page 9)

expertise in the nuclear licensing arena, will be substantially involved in shepherding the construction and operating licenses of as many as 16 or more new plants through the regulatory process for the Nuclear Regulatory Commission in the coming years. Activities will range from performing environmental reviews to evaluating fuel designs.

PNNL also anticipates contributing to the Global Nuclear Energy Partnership, a comprehensive strategy to increase U.S. and global energy security, encourage clean development around the world, reduce the risk of nuclear proliferation and improve the environment (see related story, page 15).

Demand-side Technologies

Traditionally, most of PNNL's energy business has focused on energy-efficient technologies and includes areas such as energy-efficient building and vehicle technologies. The Laboratory continues to lead development of solid oxide fuel cells (see related story below) and plays a major role in solid-state lighting. It also has an active role in the development of codes and standards for building efficiency and ongoing

work on advanced diesel engines to reduce emissions in auto engines, and is working on advanced forming and fabricating technologies to produce lightweight materials for transportation. PNNL will strengthen this demand-side area with further development of innovative and novel approaches to energy efficiency in buildings (see related story, page 14), transportation, lighting and fuel cells.

Opportunities for Growth

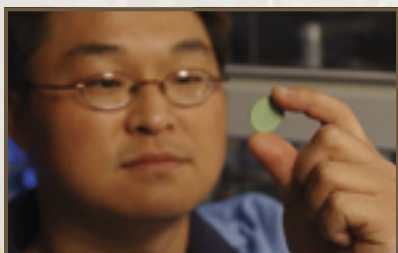
According to Virden, PNNL's energy business has grown steadily the last several years. He estimates that energy sales will total around \$93 million in 2006, up from \$65 million just two years before. "I attribute this growth to our staff staying focused on the most important problems and contributing the right solutions to solving our clients' critical challenges."

PNNL also teams extensively with industry to develop solutions. "Our industry partners are savvy as to what works in the real world," Virden said. "Working with them gives us a better perspective of industry needs and strengthens our ability to turn our science into real-world solutions."

Fuel cell prototypes exceed expectations

Fuel prices continue to rise. However, one solution—fuel cells—is gaining on that problem. The Solid State Energy Conversion Alliance (SECA) has achieved the first of a three-part goal: developing solid oxide fuel cell systems that reduce fuel cell production costs by a factor of ten.

SECA is a collaboration between industry, academia and other research organizations to develop modular, low-cost, fuel-flexible solid oxide fuel cell (SOFC) systems that



Scientists at Pacific Northwest National Laboratory are developing materials and techniques used to fabricate solid oxide fuel cells. This test of a "button" cell will help select electrode materials for full-sized cells.

can operate on coal gas, natural gas, hydrogen, and liquid fuels. SECA is led by Pacific Northwest National Laboratory and the National Energy Technology Laboratory (NETL) and funded through the Department of Energy's Office of Fossil Energy.

"With this goal accomplished, we can now proceed to the second step—refining our modular fuel cell design to make it more easily customized for diverse commercial applications," said Gary McVay, who manages PNNL's role in SECA.

Although fuel cells are considered a potential solution to the nation's energy problems, they currently are too expensive for widespread use. By developing a fuel cell for diverse applications, the SECA team intends to reduce costs. Potential applications include military, transportation and land-based power generation.

Manufactured with a scalable mass-production technique, the first-phase SOFC prototypes exceed all of SECA's Phase I targets for performance degradation, efficiency, endurance and production cost.

The SECA program involves six industry teams using varied approaches to design a fuel cell that will meet DOE cost and performance goals while also meeting their own specific needs. In addition, leading researchers in industry, academia and at national laboratories support the industry teams with cutting-edge research and development.

Coal: an energy bridge to the future

For years, coal drove the transportation business in this country, and it may be poised for a comeback. A hundred years ago, steam engines burned tons of coal as they pulled trains across the country. Now researchers are looking at converting that coal to liquid fuel to fill our gas tanks and move cars and trucks.

“With the price of gas painfully high and with the negative foreign trade balance and national security issues associated with importing oil from other countries, coal is getting more than a second look,” said George Muntean, who manages PNNL’s Energy Conversion Initiative.

The technology already exists to transform coal into a liquid fuel. In fact, Pacific Northwest National Laboratory scientists and engineers have researched forms of coal and hydrocarbon gasification on and off for more than 30 years. But oil has never sustained a high enough price to kick-start a coal-to-liquid fuel industry. That might be changing now.

Plus, experts agree worldwide petroleum resources won’t last forever, and hydrocarbon resources like coal may be the only resources available, at a large enough scale, to off-set oil consumption, in the near term.

“If coal is used cleanly and efficiently, it can serve as an energy bridge to the future in which renewable energy and nuclear and hydrogen-based energy sources will make up our energy systems,” said Mike Davis, associate laboratory director for the Energy Science and Technology Directorate.

The United States has the largest coal reserves anywhere—about one fourth of the world’s supply. But, historically, its impact on the environment has been problematic.

While the process of converting coal to a liquid is inherently cleaner than burning coal to produce electricity, there are still challenges with water usage and air emissions—especially carbon dioxide. CO₂ is implicated in global warming.

Solving the CO₂ problem is one of PNNL’s biggest strengths when it comes to utilizing coal. “We are at the forefront of research into carbon capture and sequestration,” said Muntean.

Gasifying coal releases CO₂ but also produces a very high-quality synthesis gas. The process to convert this so-called syngas to liquid fuel is called Fischer-Tropsch, after two German scientists who developed the technology in the early 20th century. It was employed, in conjunction with coal gasification, during World War II when Germany had trouble importing sufficient petroleum.

The liquid fuel produced from coal can be blended with traditionally refined fuels, used by existing diesel engines and transported and delivered in the same manner as the diesel we’re all familiar with, so no change in infrastructure is needed.

PNNL recently launched an Energy Conversion Initiative—an investment in identifying the science and technology challenges and defining the conditions for commercial success needed for economically and environmentally sound use of domestic hydrocarbons, such as coal.

In addition to the Laboratory’s expertise in carbon capture and sequestration, researchers are building on capabilities in FT synthesis, catalysis and nanotechnology, separations, materials and sensor development to make the conversion process more efficient—better, faster, cheaper—and to reduce capital costs of building coal-to-liquid production plants.



Because domestic coal supplies are plentiful, PNNL researchers are looking at whether it can be cleanly and efficiently converted to transportation fuels to replace some of the 12 million barrels of oil the United States now imports per day.

PNNL is engaged with state governments that are interested in using their coal resources for transportation fuels. PNNL hopes to create government-industry partnerships that will develop process capabilities that can be demonstrated in pilot or full-scale commercial plants within five years.

“If we can tap this domestic resource in a way that doesn’t harm the environment, we can really make a dent in the 12 million barrels of oil we import each day,” Davis said. “I believe it can be done.”

Moving grid operations from minutes to seconds

In the last century, the electric power grid has grown from a system that served one square mile in New York into a highly-complex interconnected system that serves all of North America.

Initially, individual local systems would connect to each other to share resources and increase reliability. Today, utilities rely upon that same interconnectedness to save money by shipping large amounts of power over long distances, pushing the system closer to its limits more and more often.

At Pacific Northwest National Laboratory, researchers are exploring how changes in the way the nation's electrical grid is operated can improve its reliability and effectiveness—lowering costs and lessening environmental impacts. The focus is on developing real-time tools and supporting their integration into operating systems.

According to Rob Pratt, who leads PNNL's Electricity Infrastructure Operations (EIO) Initiative, there is a

need for grid operators to see beyond the individual control areas within their purview. If operators understand what is happening on neighboring systems, they could more quickly recognize and address the potential impacts to the system they operate.

This need for "situational awareness" was a key finding following the East Coast blackout of 2003, where events leading up to the blackout could have been detected and corrected before they spun out of control. Once started, the blackout spread from Ohio to New York in only nine seconds.

PNNL's EIO Initiative focuses on improving situational awareness by collecting more and richer data from a broader area and developing tools that allow timely analyses and therefore quick and appropriate action.

For example, data collected by a conventional SCADA (Supervisory Control and Data Acquisition) system currently are refreshed only every four seconds. It can be another four minutes before the data are analyzed and results are available to operators. "Operators don't know for four minutes or more if the news is good or bad," Pratt said. However, a new and more precise type of data called phasor data that are time-stamped and synchronized could be shared with operators across the system 30 times per second.



August 14, 2003—about 20 hours before the blackout.



August 15, 2003—about 7 hours after the blackout.

Photos courtesy of NASA.

"But as we all know, having data is not enough," Pratt said. "We will eventually have thousands of these data points available, but we need new technology, including advanced analysis and visualization tools, to know where and when to look—and what we should be looking for."

Researchers are applying data-intensive computing to the process used to reconcile data coming in from the grid and the underlying fundamental physics of its operation. Called "state estimation," it takes a few minutes to develop a comprehensive picture of the grid that can be used also for contingency analysis to determine likely outcomes and potential next steps.

"By advancing the architecture and the algorithms and specifically tailoring them to the problem at hand, we've already sped up this process by an order of magnitude," Pratt said. Right now, researchers depend on high-performance computing capabilities of DOE's

Office of Science for these breakthroughs, but Pratt said it won't be long before this kind of processing will become available in mainstream systems for utilities.

The EIO Initiative also is focused on research to help understand the dynamics of the electric grid and build those properties into improved real-time models. Today's operational models assume that the grid is in a steady state, ignoring oscillatory behavior that can potentially bring it down. Current studies of the grid's dynamic stability are so slow that they're typically done offline and can't be incorporated into control processes. Without precise models, the grid is often operated with more margin than needed, which results in real economic impact.

The Initiative centerpiece is the Electricity Infrastructure Operations Center, a fully capable grid control center that serves as a platform for grid research and development, testing and training (see related story, next page).

As demand for electricity continues to grow, the existing transmission and distribution system will continue to get pushed to its limits, threatening its reliability. "We can't afford to gold-plate the grid to make it reliable," Pratt said. "Instead, we're focused on how to safely live close to the edge—knowing with confidence where that edge really is—while keeping the lights on."

Operations center is the real deal

Grid operators who spend their days managing a piece of the nation's electric grid could walk into the Electricity Infrastructure Operations Center (EIOC) at Pacific Northwest National Laboratory and feel right at home.

Complete with \$3 million in energy management system software provided by industry leader Areva T&D, secure computer networks, 30 work stations, more than 100 servers, 25 special-purpose computers and a 115-square-foot video wall, the EIOC is a fully capable control center with access to real data from North America's eastern and western power grids.

"We have created a platform for research and development that serves as a point of departure for grid operations," said Ross Guttromson, EIOC manager. "That means this facility picks up where industry currently leaves off."

By adding utility-specific grid models and SCADA data, the EIOC actually could control part of the grid just like the 130 existing control centers in North America. Its primary purpose, however, is to provide a real operations environment for researchers to develop, assess, test and deploy tools for managing the grid.

The functionality and data available in the EIOC make it possible to try out new technologies without the cost and risk of potentially negatively affecting an actual system. As a safe test bed, researchers can work more

quickly through the iterative process of developing and refining technology, which includes manufacturers, researchers and users. "I like to say you can get about 80 percent of the benefit of a full-blown demonstration for about 20 percent of the cost," Guttromson said.

Some research in the EIOC is focused on helping operators understand what's happening on neighboring systems, how it might affect their own system and what to do once they know there is a problem. "It's about understanding what you need to know at the right time and knowing what to do with it," Guttromson said.

In addition to visualization technologies and improved predictions of grid behavior, the EIOC is home to human factors research. By understanding the psychology of operators, the way they approach their jobs and their workplace culture, researchers can address those aspects in new technologies so they actually get used instead of sitting on the shelf.

The EIOC also supports operator training, exploring uniquely realistic simulations and scenarios that include failing indicators and computer hackers.

DOE and government agencies can use the EIOC to test solutions and understand the potential benefits of technologies. This facility also could be used by utilities trying to solve a

particular problem or by manufacturing companies interested in safely testing new technologies, vetting them with users and integrating them with actual data—all within the same environment where the technology eventually will be put to use.



A closer look at the Northwest hydro system

Pacific Northwest National Laboratory brought together public and private utilities, technology vendors and research institutions from across the Northwest to gather insight into challenges and opportunities for the region's power grid.

The group helped set the research agenda for the Electricity Infrastructure Operations Initiative, including identifying a desire to better manage the Northwest hydropower system. "You can't treat individual dams like separate power plants," said Rob Pratt, initiative leader at PNNL. "We have an asset that's complicated to operate and fully subscribed, given constraints in place for international treaties, fish, irrigation, transportation and recreation."

As a result of the group's input, PNNL is investing in projects designed to squeeze more out of the hydro system by improving forecasts of snowpack and runoff and developing water management tools. Probability-based forecasts and advanced optimization techniques can bring management of the hydropower system closer to real time.

"We think we can save more fish and get more power from the system by understanding the opportunities better," Pratt said.

CREATIVE ENERGY

PNNL researchers are generating real-world solutions to a global problem

PNNL's building sciences: from concept to commercialization

The Department of Energy has a new vision for residential and commercial buildings in the United States—net-zero energy buildings that will produce as much energy as they consume.

According to DOE, the building sector—including residential and commercial buildings—currently is the largest energy consumer. Through new technologies and design approaches, however, a building constructed in 2025 may be 60-70 percent more energy efficient than one built today, with the remainder of its energy needs coming from renewable technologies, such as solar and wind, or other zero-emission sources.

“Pacific Northwest National Laboratory is supporting DOE in its efforts to reach zero-energy buildings through activities ranging from basic research to developing and moving new technologies into the marketplace,” said Marylynn Placet, who oversees PNNL's work for the DOE Building Technologies Program. “Ultimately, our goal is to develop innovative approaches for buildings and help transform the market to accept them.”

Assisting government and the private sector

With a diverse staff of scientists, engineers, economists and market analysts, PNNL conducts a wide range of buildings projects for DOE and other agencies, such as the U.S. Army and Navy. For decades, PNNL has helped the federal government improve efficiency through better operating and maintenance processes, sustainable design practices, analytical tool development and other types of technical assistance. PNNL also documents best practices in residential construction, in support of DOE's Building America program, to help private-sector builders reduce energy use.

Going “high-tech”

Another one of PNNL's long-term projects involves developing and deploying sensors, diagnostics, and controls



At one of its state-of-the-art facilities, PNNL conducts organic-inorganic thin film research in the pursuit of revolutionary low-cost, efficient lighting.

to monitor and reduce energy use in buildings. Someday, buildings might be monitored and controlled with the same sophistication as today's automobiles.

Providing the science foundation

PNNL's basic research in materials science, thin film deposition and modeling serve as the foundation for a number of breakthroughs. For example, PNNL materials scientists are experimenting with biomaterials and new modular construction techniques for residences. At the molecular level, PNNL research is advancing the development of organic light-emitting diodes or OLEDs, a form of solid-state lighting that provides exceptional brightness, can be constructed with inexpensive materials and offers low energy consumption. Success in this research could transform lighting in buildings.

Helping consumers choose efficiency

In addition to the cutting-edge research in support of solid-state lighting technology, PNNL staff members are working to facilitate deployment in the marketplace. For example, PNNL is helping DOE develop ENERGY STAR® specifications and testing procedures for solid-state lighting products that will ensure that devices exhibit the kind of energy-efficient performance consumers expect. In addition, the PNNL-managed Light Right Consortium research is helping building owners understand the positive impacts on worker productivity associated with energy-efficient, quality lighting design.

Reshaping the market

Since 1991, PNNL's Building Energy Codes Program, or BECP, has delivered cumulative energy cost savings of almost \$8 billion and saved enough energy to meet the requirements of about five million homes for a year. BECP works closely with national codes organizations to develop model codes that maximize energy efficiency in cost-effective and easy-to-understand ways. In addition, BECP works with state and local governments to adopt the new model codes and develops software tools that allow builders to determine if their buildings meet the energy code.

Researchers at PNNL also are helping DOE develop energy-efficiency standards for building equipment—some for the first time. PNNL is analyzing air conditioners and heat pumps typically used in hotels; commercial refrigeration equipment, such as refrigerated and freezer cases in grocery stores; and beverage vending machines.

PNNL capabilities in materials science, mechanical and electrical engineering, building energy analysis, simulation modeling, economics and market analysis underlie much of the cutting-edge research being conducted by PNNL for the Building Technologies Program and other agencies. PNNL is helping make net-zero energy buildings a reality by 2025—or sooner.

Nuclear energy and the 21st century

The world is entering a period of renewed interest and growth in nuclear energy, driven by rising oil prices, growing demand for electricity, new passively safe plant designs, and low emissions of greenhouse gases, which some governments need to meet Kyoto Protocol standards. The Kyoto Protocol assigns mandatory targets for reducing greenhouse gas emissions to signatory nations.

Pacific Northwest National Laboratory is well positioned to be a major player in this nuclear energy “renaissance.” The Laboratory has a long history of evaluating nuclear systems, developing new technologies and improving nuclear facility operations for clients such as the U.S. Nuclear Regulatory Commission, the U.S. Department of Energy and the National Nuclear Security Administration.

A major opportunity is materializing on the horizon for PNNL to assist the NRC in reviewing and evaluating construction and operating licenses for as many as 20 new nuclear power reactors in the United States over the next decade. Ten companies have announced they will seek licenses to build new power plants in the United States. Energy Secretary Samuel W. Bodman recently announced that DOE would provide \$2 billion in federal risk insurance to companies applying to build nuclear power plants—part of an incentive package designed to encourage construction of the country’s first nuclear reactors since the 1970s.

PNNL is part of a consortium comprising four DOE Office of Science laboratories that has submitted a proposal to the NRC to provide assistance with reviewing the Combined Construction and Operating License applications for these new reactors. “Our staff has extensive nuclear licensing-related experience such as revising the NRC standard review plan for light-water reactors and operating licensing requirements,” said Al Ankrum, PNNL’s relationship manager for NRC. “We also have people with strong operations background honed from years of experience at the N Reactor at Washington’s Hanford Site, the Trojan nuclear power plant in Oregon and other nuclear plants around the country.” Currently, the Laboratory is conducting a number of environmental reviews on behalf of NRC for siting the planned new reactors.

PNNL also is well positioned to play a major role in the newly created Global Nuclear Energy Partnership (GNEP) program, a comprehensive strategy to increase U.S. and global energy security, encourage clean development around the world, reduce the risk of nuclear proliferation and improve the environment.

While the nuclear energy renaissance in the United States is just starting to unfold, “the growth in nuclear power overseas is phenomenal,” said Jon Phillips,

manager in PNNL’s International Security and Nonproliferation group. China, for example, is building two to four reactors a year, and India is constructing more than 10 civilian nuclear power reactors to meet growing demand. Other nations such as Japan, which lack natural resources, are building new reactors to meet their energy security needs, while countries in Europe are reconsidering the possibility of using nuclear power to meet carbon emission standards. “GNEP is about addressing this phenomenal growth and the challenging issues, such as disposal of spent fuel and proliferation of nuclear weapons, related to it,” Phillips said.

DOE’s Office of Nuclear Energy (NE) serves as steward of GNEP and partners with other organizations, including the National Nuclear Security Administration, which covers all aspects of GNEP’s nonproliferation objectives. PNNL plays a lead role in supporting the NNSA as it develops plans to implement the safeguard and security elements of GNEP.

PNNL also has been approved by NE to receive funding for GNEP research in 2007, according to Jim Buel, PNNL’s account manager for DOE Nuclear Energy activities. These new projects include on-line instrumentation for process monitoring and materials control and accountability, waste form development, systems analysis, fast reactor materials analysis, and sodium technology for fast reactors. Other potential opportunities include hot testing of unit operations within the separations flowsheet and remote fuel fabrication for fast reactor fuels.

“PNNL’s greatest strength is that it has capabilities spanning every single area associated with nuclear power, from nuclear engineering technology to national security,” Phillips said. “Our capabilities across the spectrum will enable PNNL to effectively serve the R&D interests of the U.S. government in meeting energy security, environmental and international security needs.”



PNNL introduces savvy new information tool

The Pacific Northwest National Laboratory has a new Web site that offers a vast array of information, both relevant and easy to access. Paired with Google search technology, the site is highly visible and provides unencumbered avenues to information on PNNL science and technology and their applications.

The new Web site incorporates four primary mission areas that highlight the Lab's commitment to research in national security, energy, the environment and fundamental science.

Commitment to PNNL's visitors, both public and private, was considered throughout the design process. Improved pages with access to technologies available for commercialization have a fresh new look and feel. The new design will allow industry professionals to navigate easily through the large number of available technologies that PNNL has to offer. Technologies are organized according to potential industry application, which enables users to focus on technologies relevant to their needs.

Beyond available technologies, the Web site offers a clearer path for doing business with PNNL. Whether contracting research projects or procuring a contract to supply paper products to the Lab, site visitors can find the information they need for a successful business experience with PNNL.

Other key features of the upgraded site interface are continuous highlights of PNNL's latest scientific



achievements, front-page access to news releases and publications, and easy-to-navigate paths to the Laboratory's research divisions.

The new Web site showcases PNNL's multi-purpose delivery of science and solutions as a tremendous asset in the Department of Energy portfolio of national laboratories. *Breakthroughs* readers are encouraged to learn more about PNNL by visiting the site at <http://www.pnl.gov>. ●

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