Breakthroughs

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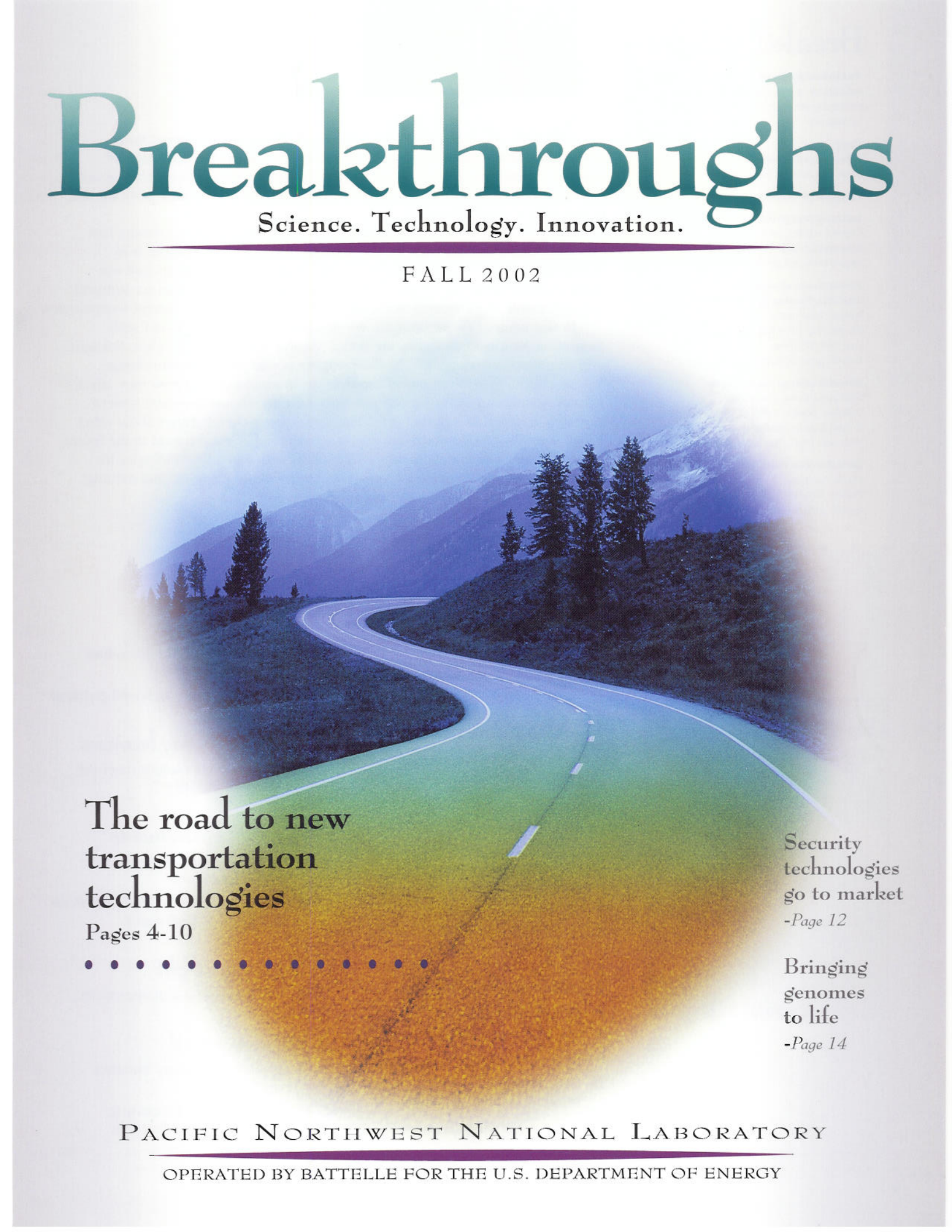
FALL 2002



The road to new transportation technologies

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PACIFIC NORTHWEST NATIONAL LABORATORY

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Breakthroughs

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editor's screen

Most of us take transportation for granted. We don't think about greenhouse gases during trips to the grocery store. We don't let fuel efficiency weigh too heavily in car buying decisions. We don't complain about the emissions from semi-trucks as much as we do about how they labor up hills ahead of us on the highway.

The government, however, is steering its attention toward increasing fuel efficiency and reducing emissions in vehicles due to concerns about how transportation affects global climate change, negative health effects and our nation's dependence on imported oil. In response, regulators have set stringent and aggressive requirements, some of which can't be met with current technologies.

In this issue of *Breakthroughs,* we describe what researchers at Pacific Northwest National Laboratory are doing to solve transportation needs. Scientists and engineers are studying vehicles' contributions to global climate change, learning about specific chemical components in emissions and how they affect human health, and exploring technologies such as exhaust treatment systems, lightweight materials and fuel cells. This issue also includes stories about other PNNL research and development that is accelerating down the road to the future. Some highlights include licensing a suite of security-related technologies for commercialization, launching a new homeland security initiative, and earning an R&D 100 Award for bioinformatics software. ●

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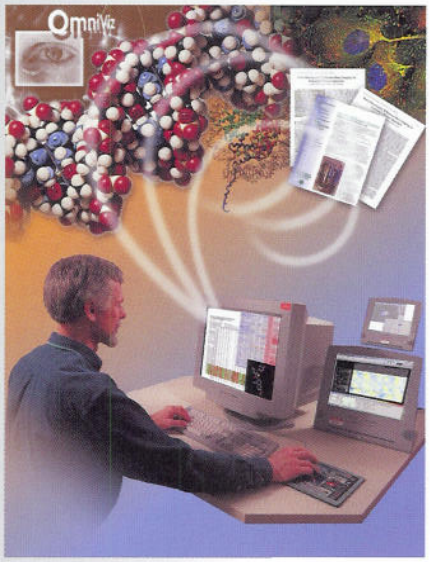


Something fishy?

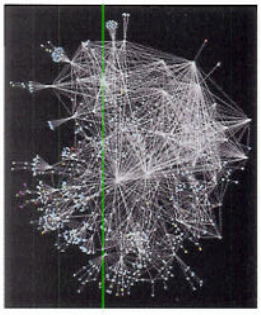
Pacific Northwest National Laboratory researchers are analyzing fish from about 500 randomly selected lakes and reservoirs across the country for ultra-low, trace levels of mercury and for specific forms of arsenic. The project is focused on freshwater game fish, such as lake trout, and bottom-dwelling fish, such as catfish. It is part of the National Fish Monitoring Study and is being performed through a contract between the Environmental Protection Agency (EPA) and Battelle, which operates PNNL for the U.S. Department of Energy.

Mercury has been detected in all of the 400 fish researchers have analyzed two years into the four-year study, while arsenic levels have been extremely low or nondetectable. "Mercury is a relatively high risk in some freshwater fish, depending on the species, age and body of water," said Eric Crecelius, PNNL program manager for the study.

When the study is complete, the EPA will send the data to individual states, which will use it to make decisions about the health risks of freshwater fish in specific bodies of water. ●

Mozart—A genius at assessing your Web site

Based on new risks posed by adversaries seeking strategic information available on the Internet, government agencies and industry have been combing through their Web sites to remove sensitive information. The task is time consuming and potentially expensive. But thanks to an Internet assessment tool under development at Pacific Northwest National Laboratory, a thorough analysis soon will be just mouse clicks away.



The tool, called Mozart, quickly archives and analyzes entire Web sites based on search terms provided by the user and built-in search libraries containing hundreds of key phrases designed to find sensitive information. The output is a hyperlinked report, including a prioritized listing of Web pages containing potentially strategic or sensitive information both within the user's organization and at externally linked sites.

This information also is presented in a three-dimensional, graphic representation. PNNL is interested in working with government and industry partners on continued development of Mozart. ●

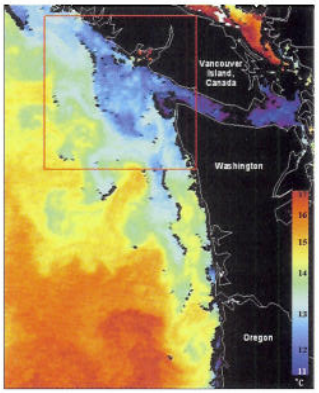
Detecting and monitoring harmful algal blooms

Scientists at Pacific Northwest National Laboratory's Marine Sciences Laboratory in Sequim, Wash., are working with the Olympic Region Harmful Algal Bloom (ORHAB) project to investigate the mechanisms driving harmful algal blooms.

Harmful algal blooms (HABs), a common occurrence on the Washington coast, have led to closures of commercial, tribal and recreational shellfish harvest, which have resulted in millions of dollars in losses to the state's razor clam fishery in recent years. Currently not enough is known about how HABs spread to predict the location and frequency of shellfish contamination along the coast.

PNNL scientists are using satellite imagery of sea surface temperatures and chlorophyll concentrations, coupled with monitoring data to better understand where and when blooms occur. The long-term goal is to develop a forecast tool that can advise coastal resource managers and tribes of HAB events.

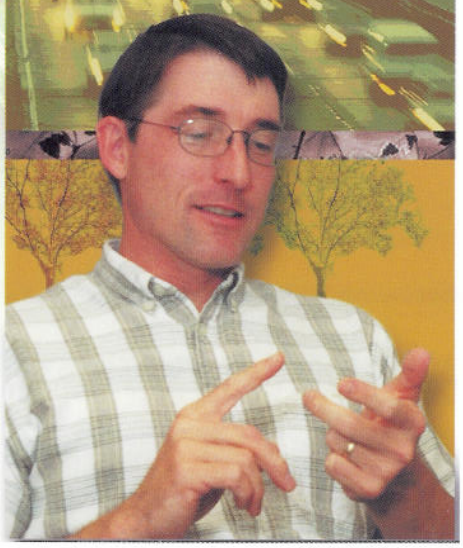
ORHAB is sponsored by the National Oceanic and Atmospheric Administration and led by the National Marine Fisheries Science Center. ●



The Juan de Fuca eddy, shown as cooler (blue) water in the outlined box, is thought to be a potential initiation site of harmful algal blooms along the outer Washington coast.

special REPORT

Need for transportation technologies heads into overdrive



The transportation industry faces several challenges relating to vehicle fuel efficiency, regulated emissions and global warming. We talked with Pacific Northwest National Laboratory's Jud Virden, deputy director for the Energy Science and Technology Directorate, about technologies being developed for transportation and how they fit into the nation's priorities relating to petroleum imports, global climate change, and environmental and health effects of emissions. Virden oversees the Laboratory's involvement in the U.S. Department of Energy's FreedomCAR and Vehicle Technologies program and other vehicle technology research.

What critical issues face transportation?

We Americans love to drive cars. Cars are part of our culture and will continue to be in the foreseeable future. With more than 200 million cars and trucks registered in the United States and an additional 15 million new automobiles sold each year, the transportation sector is increasingly dependent on imported petroleum as fuel. The U.S. produces only one third of the petroleum we consume. In light of the events of September 11, the growing gap between the petroleum we produce and the petroleum we consume has added significance. While great gains were made in automobile fuel efficiency in the 1980s, over the last 10 years more people are buying less fuel-efficient sport utility vehicles, mini-vans and trucks, including me. We have to balance our love for big vehicles and the increase in foreign oil we consume.

Another critical issue is the release of regulated emissions such as carbon monoxide, oxides of nitrogen and particulate matter. It's amazing that total emissions from all vehicles have decreased over the last 30 years, even though the number of registered cars, trucks and buses has almost doubled. The auto industry has done a great job optimizing engine control, including introducing computer controls, and reducing emissions with three-way catalysts. But this is only the beginning, especially for heavy trucks. Diesel-powered trucks, ships and trains are the backbone of our economy, which depends on efficient and timely movement of freight. Over the last 25 years, the oxides of nitrogen and particulate matter emissions from heavy trucks—the 18-wheelers you see on the highway—have been reduced by 90 percent. New regulations that take effect in 2010 require another 90 percent reduction in tailpipe emissions. This is a monumental task.

The impact of emissions on human health is another major issue. In recent reports, diesel particulate has been singled out as a carcinogen. There is much debate around these reports, but to me, the important question is how far do we need to reduce emissions before the impact on human health is acceptable? We need a better understanding and correlation between human health and what comes out of the tailpipe. This requires more data on vehicle emissions, how they are transported through the atmosphere and their impact on human health.

The final critical issue is the transportation sector's impact on global warming. Carbon dioxide is a greenhouse gas that contributes to global warming, and the amount released from the transportation sector is growing steadily. Transportation accounts for about a third of the carbon dioxide released, with 473 million metric tons of carbon released in 1997. For cars and trucks, which use carbon-based petroleum fuels, the best way to reduce carbon dioxide is to reduce fuel usage or increase fuel efficiency. If one gallon of fuel can take you farther, less carbon dioxide is emitted.

How did PNNL's research in this area begin?

In the mid-90s, we began materials research and developing lightweight materials as part of the Partnership for New Generation Vehicles, or PNGV, a government program that included Ford, General Motors and Chrysler. The program focused on increasing fuel efficiency in light-duty vehicles such as passenger cars and included a goal to reduce the weight of vehicles by 50 percent.

At the suggestion of PNGV, this Laboratory initiated the Northwest Alliance for Transportation Technologies in 1996. It focuses on engaging the region's producers of aluminum, magnesium, titanium and polymer composites in research and development to support the transportation industry. At that time, Washington and Oregon were responsible for more than 40 percent of domestic aluminum

production. PNNL's programs have continued to grow and now include Alcoa and Delphi Corporation, and Northwest-based heavy truck producers, PACCAR and Freightliner. Today we have expanded our program to include emission reduction, solid oxide fuel cells and health effects research.

How do the needs of lightweight vehicles and heavy-duty trucks differ?

Heavy truck purchases are primarily a business decision. Initial cost and operating cost versus the payback period are critical. A new heavy truck costs more than $100,000 and some run 16 hours a day, most days of the year. A fleet owner or independent trucker purchases a truck to make money, so fuel prices and vehicle efficiency are important. They expect trucks to be reliable, durable and cost effective for at least 400,000 miles. Over its life, a heavy truck may end up going more than a million miles.

Personal vehicles are a different story. Most of us buy vehicles based on personal preferences and emotion. The initial cost is very important to us, but operating cost is not usually a major consideration. Surveys show reliability and safety are high priorities for new car buyers. Fuel efficiency is not. Personal vehicles are expected to last about 100,000 miles, which is when typical car owners are ready for something new.

While both heavy trucks and personal vehicles require cost-effective, reliable and durable technologies, there are some major differences in the technologies needed for each. Heavy vehicles are primarily diesel powered while cars are primarily fueled by gasoline. Perhaps the biggest difference, however, is in product volume and cost for new technologies. Each year, the number of heavy trucks manufactured is about a couple hundred thousand, compared to about 15 million personal vehicles. New technologies for trucks can be produced in low volume but must be reliable for several hundred thousand miles. New technologies for cars must be manufactured in very high volumes and last at least 100,000 miles or 10 years.

What are PNNL's areas of expertise?

We have the right fundamental science foundation to contribute in several critical areas. This includes strengths in materials science, chemistry, ceramics, interfacial and surface science and modeling. We also have unique equipment and facilities.

But having the right science isn't enough if it can't be translated into actual applications. We form interdisciplinary teams that work on basic and applied research, building the scientific understanding needed to direct research toward solutions. We have demonstrated that we can develop new concepts, move the technology to pilot-scale demonstrations and address manufacturing issues. Most importantly, our new technologies focus on industry needs.

For example, superplastic forming methods developed at PNNL allow more complicated shapes to be manufactured in less time and with fewer parts. While lightweight materials themselves may be more expensive than traditional materials, the overall cost of raw materials and fabrication is reduced.

What is PNNL's focus?

We're working on lightweight materials, emission reduction technologies and fuel cell technologies, including developing solid oxide fuel cells for auxiliary power units in vehicles.

Fuel cells could provide exactly as much power as long-haul trucks need to sustain their "hotel load." With the help of a fuel cell, a truck's refrigeration unit, lights, heat or air conditioning for the cab, a power source for computers and cell phones, and other power devices could operate during rest stops without the engine running. Today, truckers run a 600-horsepower engine to provide the few kilowatts they need during stops. Due to concerns about truck emissions, there is pending legislation that would prohibit trucks from idling on the side of the road. Fuel cells could be a solution.

Our researchers are working on ways to put fuel reformers onboard vehicles so various kinds of fuel, including diesel, could be converted into the hydrogen gas needed to operate a fuel cell. Through our involvement in the Solid Energy Conversion Alliance, we're working on fuel cell technologies with industry partners, including Delphi, McDermott, Honeywell and Cummins.

We also are excited about our role in understanding and developing advanced catalysts for treating diesel engine exhaust. While diesel engines are more efficient than gasoline engines, they pose different challenges. Diesel engines run lean, meaning there is excess air in the exhaust. In those conditions, different catalysts are needed to reduce oxides of nitrogen, and particulate matter emissions. Almost every technology for reducing emissions decreases fuel efficiency, but the goal is to reduce emissions without a "fuel penalty." Our researchers are working with engine manufacturers and catalyst suppliers to develop new systems that will help industry meet future emission standards.

How does the Laboratory work with industry?

DOE's FreedomCAR and Vehicle Technologies program and the Hydrogen, Fuel Cells, and Infrastructure Technologies program are the primary sponsors of our projects, along with industry partners that help fund our research. By teaming with industry, the answers we provide with scientific research are applicable to industry and actual applications. In addition to the key partnerships already mentioned, we work with Caterpillar, Detroit Diesel and many others. Our industry partners provide direction that focuses our research, including projects that have earned national awards and recognition.

Partnerships with industry have been a common theme throughout our research related to transportation and vehicles. Through these partnerships, we expect our technologies to impact the future. ●

Exhaustive research on emissions technologies

In a time when regulators are demanding reduced emissions from the transportation sector, Pacific Northwest National Laboratory is conducting fundamental scientific research that could help vehicles clean up their act.

Vehicles contribute heavily to four of the air pollutants monitored and regulated by the Environmental Protection Agency—hydrocarbons, carbon monoxide, oxides of nitrogen and particulate matter. The EPA's aggressive requirements for diesel engines in heavy-duty trucks include a 90 percent reduction in particulate matter emissions by 2007 and a 90 percent reduction of oxides of nitrogen, also known as NO_x, by 2010. NO_x reacts with the hydrocarbons in the atmosphere to form ozone, a major component of smog.

Industry is considering several approaches to meeting the stringent requirements because no widely applicable technology exists to solve the problem. "Industry is constantly changing requirements and preferences. But interestingly enough, the science doesn't change," said George Muntean who oversees the Exhaust Emission Science Laboratory, a program that integrates emissions research at PNNL. "Our research is applicable regardless of which emission treatment technology comes out on top."

Many technological approaches to reducing emissions rely upon delivering a "reductant" to the exhaust stream that chemically reacts with harmful NO_x molecules. NO_x forms when harmless oxygen and nitrogen in the air are exposed to the high temperatures in combustion engines. A reductant is a molecule that aids in converting NO_x back into components of clean air—nitrogen, oxygen and water.

"There are a lot of applications built around this principle," Muntean said, "but we're looking at them from the same general perspective." Researchers are striving to improve the selectivity of the reductant, which would make it more effective. They also are applying their expertise in surface science to understand what happens on the surface of the catalyst where the reaction between NO_x and the reductant takes place.

"Think about it," Muntean said. "There are no moving parts. The gas goes in dirty, flows over a large surface area material, and comes out clean. It's the surface that affects performance." Researchers need to know how molecules lay on the surface, how they interact with the surface and how the surface changes. With this understanding, they can go about preventing things that reduce the catalyst's effectiveness, such as sulfur in the exhaust blocking active reaction sites or high temperatures causing the surface to deteriorate.

The Laboratory is working with key industry partners on different aspects of these challenges. For example, through a cooperative research and development agreement (CRADA) with Caterpillar, researchers are developing a sulfur trap that potentially could be used with heavy-duty diesel engines. The sulfur trap removes the sulfur in exhaust that poisons the catalyst used to reduce NO_x.

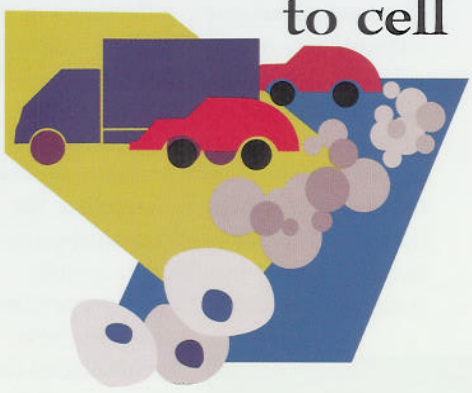
A CRADA project with Cummins focuses on NO_x adsorbers, which act like a sponge to adsorb and then dispose of NO_x. PNNL is working on preventing the adsorbers from deactivating in the presence of sulfur.

Teaming with Detroit Diesel, PNNL is investigating another exhaust aftertreatment alternative called urea selective catalytic reduction. In this approach, urea is broken down into ammonia, which is used as the reductant to strip oxygen from the NO_x molecules. While this technology has been used in stationary power production plants, it hasn't made its way to mobile applications such as heavy-duty trucks.

To address particulate matter emissions, researchers also are studying fundamental processes that affect how particulate matter, or soot, gets captured on the surface of a filter or particulate matter "trap." After the particulate matter in diesel exhaust is captured, it is burned to renew the filter surface. Researchers are addressing technical hurdles, such as preventing the filter from plugging, cracking and melting as well as improving size, cost and performance.

"At the end of the day, the device doesn't matter, because our part is the same," Muntean said. "The different approaches may seem like they have nothing in common, while in reality, the same science is behind them all."

From source to cell



By integrating its emissions research, Pacific Northwest National Laboratory scientists are focusing on emissions concerns in a broader context.

"We're building a comprehensive understanding of the problem—a source-to-cell approach," said

Opportunity NO_x

Laboratory's cornerstone technology in emission reduction

Pacific Northwest National Laboratory researchers put their expertise in surface science and catalysis to work when they developed an effective plasma catalysis system for treating engine exhaust—one of the first advanced emissions control technologies developed by the Laboratory.

This technology combines an electrically energized gas, called plasma, with a specialized catalyst material to convert oxides of nitrogen (NO_x) into components of clean air. Researchers began developing vehicle emission reduction technologies in the early 1990s, with funding from a government program focused on improving fuel efficiency and reducing emissions in light-duty vehicles.

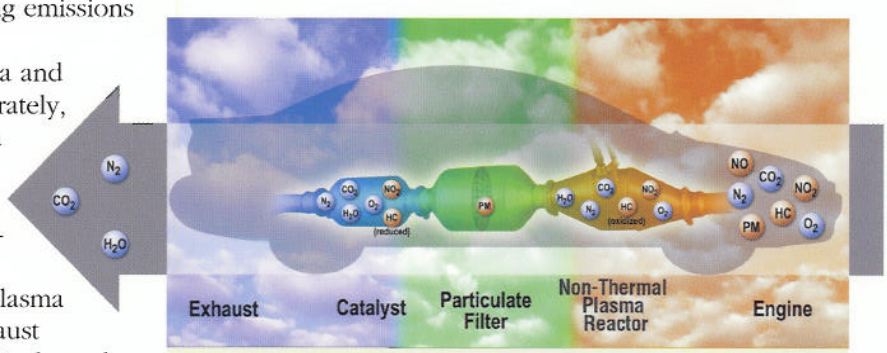
After trying plasma and catalyst methods separately, PNNL scientists took a unique approach. They combined the techniques into a two-phase process that applies non-thermal plasma processing to the exhaust stream before passing it through a specialized catalyst system. In laboratory tests, PNNL's non-thermal plasma catalysis for engine exhaust treatment reduces NO_x emissions by as much as 90 percent.

"This concept of using a non-thermal plasma to activate catalysis has only existed for about seven or eight years," said PNNL's Chuck Peden, who leads interfacial chemistry and engineering research. "Today, it is recognized as a potential commercial solution."

The specialized solid catalyst developed at PNNL to optimize chemical reactions that reduce NO_x in plasma catalyst systems won an R&D 100 award in 2001, recognizing it among the top 100 technology advances of 2000.

The catalyst since has been fine-tuned even further and PNNL researchers are working with Delphi Corp. on designs for a commercial product based on non-thermal plasma technology. Delphi and PSA Peugeot Citroën have been developing a non-thermal plasma system specifically designed for Peugeot vehicles.

Researchers also are working on reducing the system's power requirements. This is important because most emission reduction technologies negatively impact fuel efficiency. "The more efficient the system is, the less impact there will be on the operation of the vehicle, and therefore, the more transparent it will be to the consumer," said Darrell Herling, a senior development engineer. ●



PNNL and industry collaborators have developed a system that converts harmful oxides of nitrogen in vehicle exhaust into components of clean air. Vehicle exhaust, loaded with nitric oxides, flows into the non-thermal plasma reactor, where it is converted into nitrogen dioxide. A catalyst is then responsible for a chemical reaction that reduces nitrogen dioxide into harmless nitrogen gas. An optional filter also reduces particulate matter. PSA Peugeot Citroën installed this system in their Peugeot 206 environmental demonstration vehicle.

Bill Pennell, director of the global environmental change group at PNNL. The idea is to understand how emissions are created and released, what happens to them once they are in the environment and how they eventually may affect human health.

To address air quality concerns, researchers are studying atmospheric chemistry, meteorology, and the fate and transport of emissions. For example, PNNL is collaborating with other national laboratories to understand the differences in atmospheric chemistry across the United States. They are finding that different strategies to improve air quality may work better in different locations due to variances in the primary sources of emissions and existing natural conditions that influence atmospheric chemistry such as vegetation, temperature and terrain.

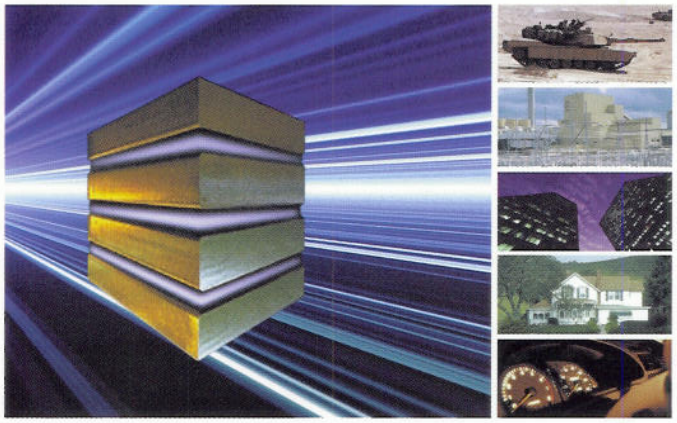
Global climate change presents a larger and longer-term challenge than traditional air quality issues. Even if all emissions stopped today, the concentration of carbon dioxide in the atmosphere would remain virtually the same for centuries and continue contributing to global climate change.

Scientists have developed new tools to look at the specific chemical composition of particles from diesel and other emission sources and how they change in the atmosphere. "We hope to determine more precisely which components of combustion do the most environmental harm," said Steve Colson, who leads this research.

A team of physical and biological scientists is studying the health effects of emissions. They are observing the biological reaction that occurs when aerosol particles are inhaled. This research includes direct visualization of lung cells as they pick up and respond to the particles. Relying on a combination of magnetic resonance imaging data and an advanced mathematical simulation of the lung, another project is looking at how particles are deposited in the lungs.

Ultimately, emissions research could lead to changes in future environmental regulations and policies relating to emissions from transportation and other sources. Rather than enforce blanket restrictions, requirements could become more focused on individual sources scientifically known to be responsible for particular environmental and health effects. ●

Fuel cells for transportation



Within five years, luxury cars and recreational vehicles on the showroom floor may be equipped with solid oxide fuel cells. That's the prediction of Subhash Singhal, director of Pacific Northwest National Laboratory's fuel cell program. Fuel cells will use the vehicle's existing fuel supply to provide auxiliary power for creature comforts, such as air-conditioning, keeping drinks cold in mini-refrigerators and viewing DVDs—all without running the vehicle's engine or draining its battery.

Fuel cells also could power refrigeration units in semi-trucks during rest stops, instead of idling engines which is responsible for about 90 percent of a semi's emissions.

PNNL is developing solid oxide fuel cells (SOFC) for military applications, such as powering individual soldier's equipment, as well as for commercial power plants, distributed generation for residential and commercial use and auxiliary power units for public and personal transportation. SOFCs also may be clustered for large-scale stationary power generation.

Similar to batteries, SOFCs convert chemical energy into electrical energy. However, fuel cells never require charging and don't run down as long as a fuel supply is available. SOFCs are fuel flexible, meaning they can use a variety of fuels, including natural gas, gasoline, diesel or hydrogen.

"Not only can SOFCs use traditional fuels, with the absence of a combustion process the fuel is used more efficiently with little to no emissions," Singhal explained. Once fuel cells are in place, combustion engines would be used solely for driving the vehicle. PNNL and Delphi Corp. have successfully demonstrated an auxiliary system for a BMW sedan that required no major modifications to the vehicle.

A team approach

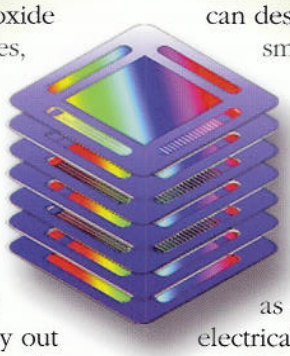
PNNL helps lead the Solid-State Energy Conversion Alliance (SECA), an alliance of U.S. industry, universities and other research organizations. Its goal is to create an SOFC technology by 2010 that will offer a low-cost, high-efficiency system for less than $400 per kilowatt for stationary, transportation and military applications.

The National Energy Technology Laboratory coordinates SECA's Industrial Teams, which develop SOFC systems for specific markets and products. PNNL coordinates SECA's other key area, the Core Technology Program, which provides technical solutions to overcome barriers identified by the industrial development teams.

"Relying on the 40 to 60 percent increase in fuel efficiencies of individual electric systems powered by fuel cells, the U.S. can extend the use of fossil fuels, reducing dependence on imported oil," said Prabhakar Singh, who manages and directs the Core Technology Program for PNNL. ●

Modeling for success

Pacific Northwest National Laboratory's unique approach to computational modeling with solid oxide fuel cells combines computational chemistry codes, computational fluid dynamics and computational mechanics. It allows PNNL researchers to study not only the electrochemical reactions in fuel cells, but also how the electrochemical reactions interact with fuel cell design.



Computational modeling is used with fuel cell development both on a global level and on the microstructure level. "The success of fuel cell programs relies on the big picture, but we also try out things to tailor the microstructure and get the behavior we need," said Moe Khaleel, who manages the computer modeling team working on fuel cells at the Laboratory. "On the global level, we look at what electrochemical reactions happen, where and at what level. From this we can design manifolds, channel heights, materials and smooth things out so we have a more reliable fuel cell system."

Using system-level modeling, PNNL researchers also predict overall system performance and evaluate controllers for the various components in the fuel cell system. They test operating conditions to improve fuel usage to make sure that the fuel cell is using as much hydrogen as possible and to yield steady electrical output during all phases of operational cycles.

Researchers also look at the fuel cell's anode, cathode and triple-phase boundary using electrochemical analysis tools to optimize microstructure performance. ●

Cooking up a better cathode

Steve Simner is like a chef, fine-tuning the ingredients and how they're assembled to find the right recipe for a new cathode material for solid oxide fuel cells (SOFC). As a material scientist at Pacific Northwest National Laboratory, his goal is to find a cathode material that will produce high power in the range of 600 to 800 degrees Celsius—low compared to the more typical SOFC operating temperature of 1,000 degrees Celsius.

"There are two fundamental goals for any cathode. The first is long-term stability and the second is high performance," Simner said. "But without stability, performance is of little consequence."

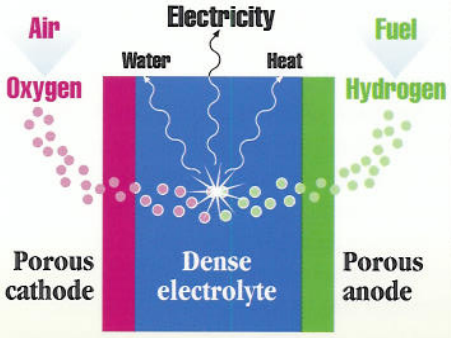
Simner's research focuses on a lanthanum strontium ferrite material, which has shown good stability in lab tests. Fuel cells using the ferrite cathode are performing two to three times better than more conventional cathode compositions.

Researchers now are trying to manipulate the composition—both physically and chemically—to further enhance its cathodic activity. "Our current composition performs well at 700 to 800 degrees Celsius, but we'd like to drop the operating temperature even further," Simner said. Lower temperatures would make it possible to replace expensive subsidiary ceramic components with more economical metal alloys. The challenge, however, is that the cathode's electrocatalytic activity decreases as temperatures go down.

Researchers are attempting to engineer structured interfaces to increase the effective contact area between the cathode material and the electrolyte. More contact area would make more reaction sites available for the oxygen reaction that takes place on the cathode side of the fuel cell.

Chemically, researchers are making subtle changes to improve material properties at lower operating temperatures. Cathodes need high electronic and ionic conductivity and the interface between the cathode and the electrolyte should readily allow oxygen transfer processes.

"We try to manipulate the chemistry of the cathode and its interfaces to enhance these properties," Simner said. He and his colleagues are adding transition metals such as cobalt to the base composition, which may improve conductivity. They also are exploring materials that may enhance oxygen transfer at the cathode-electrolyte boundary. ●



A solid oxide fuel cell is an electrochemical energy conversion device that uses conventional fuels to produce electricity. Fuel cells consist of two electrodes—an anode and a cathode—sandwiched around an electrolyte. Hydrogen from the fuel passes over the anode. Oxygen from the air passes over the cathode, gaining electrons at the interface with the electrolyte. These oxygen ions pass through the electrolyte and react with the hydrogen from the anode to form electricity, water and heat.

New anode material bodes well

Pacific Northwest National Laboratory scientist Olga Marina is developing a new generation of non-metallic anodes for solid oxide fuel cells and she is seeing promising results. With support from the U.S. Department of Energy's Office of Fossil Energy, her work is part of a significant international research effort to identify alternatives to nickel in solid oxide fuel cells.

In a fuel cell, the anode facilitates the reaction between hydrogen, carbon monoxide and hydrocarbon fuels with oxygen ions that permeate the electrolyte from the cathode side. An ideal anode should have high electrical conductivity and electrocatalytic activity, and it should be tolerant to intermittent air exposure and sulfur-containing compounds in hydrocarbon fuels such as gasoline, diesel and natural gas.

Traditionally nickel is used in solid oxide fuel cell anodes because it has excellent electrical conductivity and electrocatalytic activity; however, it also has some drawbacks that can lead to deactivation and reduced fuel cell performance. Nickel oxidizes rapidly and may break apart when exposed to air, which can occur during startup and shutdown of the fuel cell system. Nickel also is susceptible to poisoning when exposed to low concentrations of sulfur and promotes a buildup of carbon under certain conditions.

While metal oxides provide better oxidation resistance and sulfur tolerance than metal anodes, these benefits usually come at the expense of significantly lower electrical conductivity and reduced electrochemical activity.

A material that offers a good compromise seems to be the solution and Marina may have found just that. She discovered a new class of materials that provides a good balance among the many anode performance criteria. The composite composed of oxides of strontium titanate and ceria provides excellent oxidation resistance and sulfur tolerance, has electrocatalytic activity comparable to nickel and offers adequate electrical conductivity.

"It's a breakthrough because up until now there has been no good alternative to nickel. This material shows promising performance quite comparable to nickel," Marina said. The metal oxide composite outperforms any other known non-metal fuel cell anode and was announced in July at the European Fuel Cell Forum held in Lucerne, Switzerland. A patent is pending on this invention. ●

New lightweight materials produce cars of the future

Cars and trucks may be losing weight soon thanks to continuing research in lightweight materials and manufacturing technologies at Pacific Northwest National Laboratory.

Almost half of all new vehicles sold in the United States are pickups, sport utility vehicles and vans. On average, they weigh more than cars, are less fuel-efficient and present safety problems when they collide with lighter vehicles. Because these vehicles also consume the most fuel, the use of lightweight materials is expected to improve their fuel economy.

Lightweight materials and manufacturing technologies also may play an important role in President Bush's FreedomCAR program, which emphasizes a long-range shift from a fossil fuel-based transportation economy to a hydrogen-based transportation economy that uses fuel cells rather than combustion engines. But to maximize driving range and performance, hydrogen fuel cell vehicles will have to be as light as possible.

"The new focus on hydrogen means an even stronger, more urgent need for lightweight vehicles. We are redoubling our efforts in the materials sector to lighten the load to maximize hydrogen's benefits," said Mark Smith, who leads the materials resources group for PNNL.

PNNL's research extends beyond work in the lab to develop novel materials. "Our expertise in materials science and advanced manufacturing techniques gives us the means to focus on developing new lighter weight materials that also are economical to manufacture," Smith said. "The Lab's computer modeling expertise allows us to simulate the material behavior through the manufacturing process, and then see how well these materials will work on a vehicle even before building a prototype."

PNNL and the Northwest Alliance for Transportation Technology (NATT), in partnership with DaimlerChrysler, the Department of Energy's Office of Heavy Vehicle Technologies; and Alcoa, the world's largest aluminum producer, recently completed a project that involved developing three prototype lightweight vehicle frames. The prototypes, which are steel and aluminum hybrids, will be tested on the chassis of a 2002 Dodge Durango at the DaimlerChrysler proving grounds later this year.

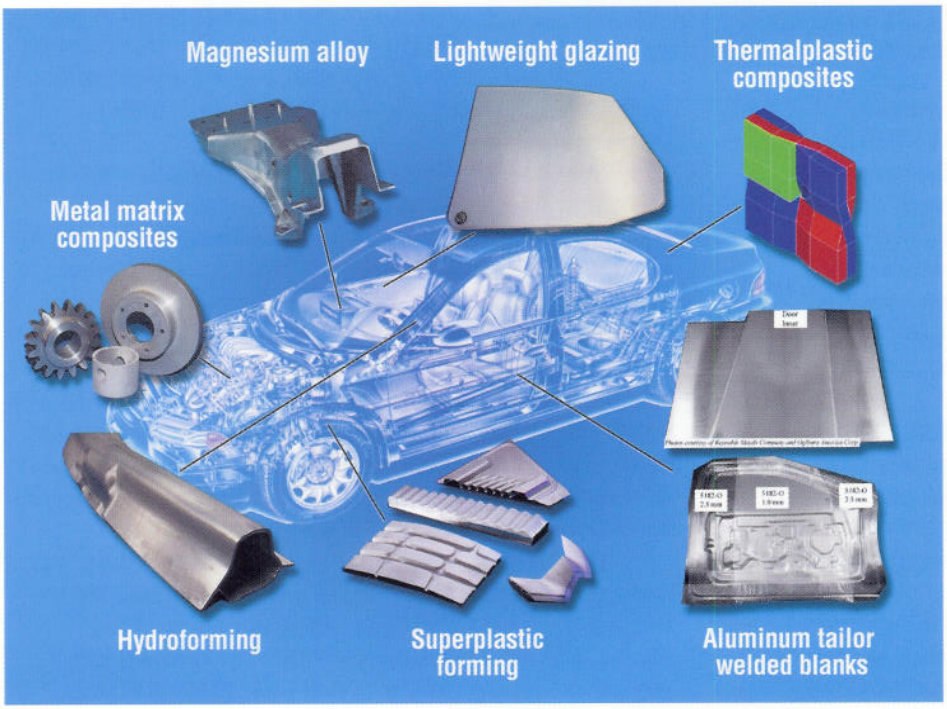
"We did not quite meet our goal of 30 percent weight reduction, but we came very close," Smith said. "If performance tests are successful, they should give DaimlerChrysler enough confidence to consider these materials in new vehicle development."

Glass, which accounts for about 100 pounds on the average family sedan, is another focus. PNNL and its automotive and glass manufacturing partners have developed a prototype windshield that is 30 percent lighter than current windshields and retains key optical, thermal and safety properties.

In the coming year, glass research will focus more on special coatings, such as those that reflect infrared rays, and will move beyond windshields to address side and rear windows.

Finally, PNNL is working on six projects with three of the major heavy-duty truck manufacturers to reduce the weight of tractor-trailer combinations by 20 percent or about 6,000 pounds. "Our goal is to increase fuel efficiency and utility of the vehicle by allowing greater payloads where needed. We want to facilitate the use of lighter weight, higher strength materials on heavy-weight vehicles, but we want to do it economically," Smith said. ●

■ **http://natt.pnl.gov/**



Byproducts and biomass fuel new opportunities

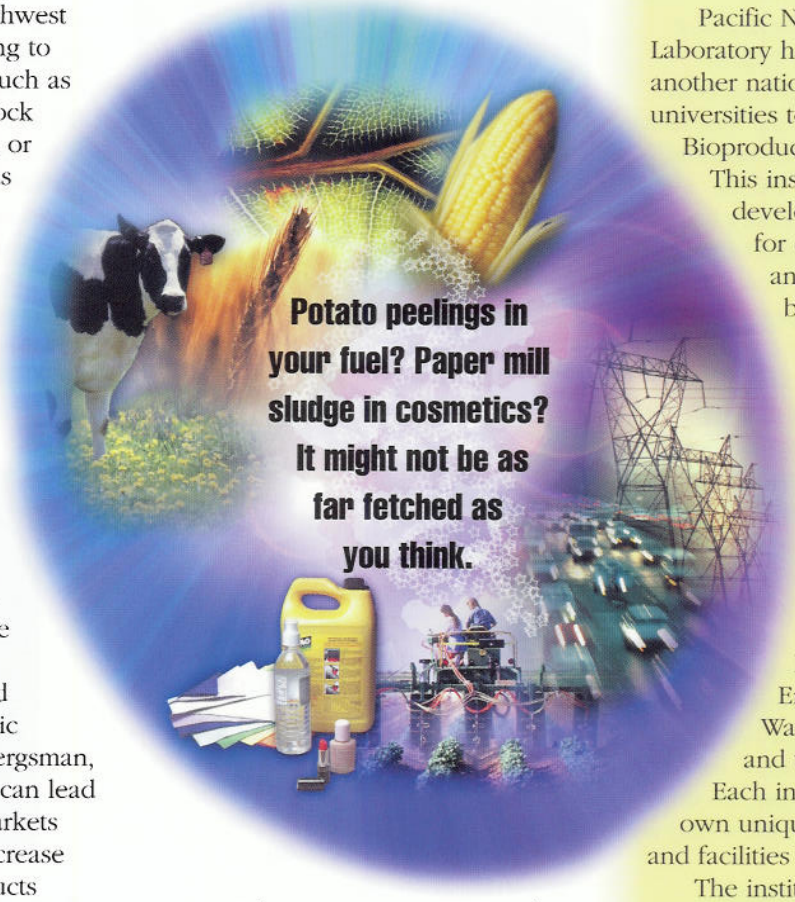
Researchers at Pacific Northwest National Laboratory are working to transform low-value biomass such as corn fiber, mill feed and livestock waste into specialty chemicals, or high value bioproducts, such as plastics, fibers, adhesives and solvents. These bioproducts often can be made less expensively than the same products made from petroleum using processes that are more energy efficient and environmentally friendly.

Biomass refers to organic materials made by living things. Examples of biomass include food processing byproducts, farm residues and waste, and byproducts from the pulp and paper industry.

"Development of bio-based products has very real economic impacts," explained Theresa Bergsman, program manager at PNNL. "It can lead to new and more profitable markets for the agricultural industry, increase the value of low-value byproducts currently used for animal feed and turn wastes such as pulp mill sludge into assets like high-value chemicals, fuels and energy. Using a renewable feedstock can help reduce our nation's dependency on foreign oil."

PNNL has been conducting bio-based products research since the mid-1970s. The hallmark of PNNL's research has been novel catalytic processes that convert sugars and organic acids to higher value commodity and specialty chemicals. PNNL also is developing a specialized capability in fungal bioprocessing.

Now the Laboratory is pulling its suite of capabilities and technologies together under a new Bio-based Products Initiative to provide a more strategic focus to addressing these issues. "Our goal is to develop a portfolio of bio-based products technology and facilitate the commercialization of this technology," explains Bill Farris in PNNL's technology commercialization group. "We need to quickly move these innovative processes from the laboratory into the marketplace." Several collaborative partnerships already have been formed with organizations such as the National Corn Growers Association, the Iowa Corn Promotion Board, Pendleton Flour Mills and Mennel Milling.



In support of this endeavor, PNNL is looking to establish a Bioproducts Processing Laboratory. This multi-user facility will include a "biorefinery" test system; extensive analytical capabilities; and biological science, chemical processing science and engineering development laboratories. When established, the Bioproducts Processing Laboratory would be capable of swiftly turning scientific discoveries into commercial technologies. ●

■ **www.pnl.gov/biobased/**

Special thanks to contributing writer, Lisa Brown

Partnerships for ag-based products

Pacific Northwest National Laboratory has teamed with another national laboratory and two universities to form the Northwest Bioproducts Research Institute. This institute will facilitate development of new methods for converting agricultural and food processing byproducts and wastes into commercially valuable bio-based energy and industrial products. The institute will emphasize maximizing the value of the products produced, ensuring long-term economic viability.

In addition to PNNL, the participants are Idaho National Engineering and Environmental Laboratory, Washington State University and the University of Idaho. Each institution will bring its own unique capabilities, staff and facilities to the group.

The institute will help to more fully exploit the productivity of American farms, which already are the most productive in the world. It will explore new uses for food processing byproducts, including discarded culls, hulls and peelings and for farm residue such as straw or manure. Currently the typical market for many of these residues is livestock feed, which provides a low economic return to the producer. In some cases, these residues can become a financial liability if they require disposal.

Industry, processors and growers will be able to use and profit from the institute's products and technologies and, in some cases, will profit from the discoveries through licenses. ●

■ **www.pnl.gov/news/2002/02-19.htm**

Science of doing business

Security technologies meet the needs of industry

A device that can identify contents in sealed containers and a system that can diagnose engine problems while the equipment is in operation are among several innovative technologies developed for national security applications that Pacific Northwest National Laboratory has recently moved into the marketplace.

Not only does PNNL conduct scientific research on important areas such as energy, the environment, national security, information technology and health, it also makes an effort to commercialize technologies so that they can help solve critical problems for industry and society.

"We're involved in every aspect of this process, from creating, identifying, evaluating and protecting intellectual property that could be commercialized, to helping promising technologies mature and eventually become deployed through licensing agreements or the creation of new ventures," said Gary Morgan, commercialization manager for PNNL's National Security Directorate.

Examples of recent matches:

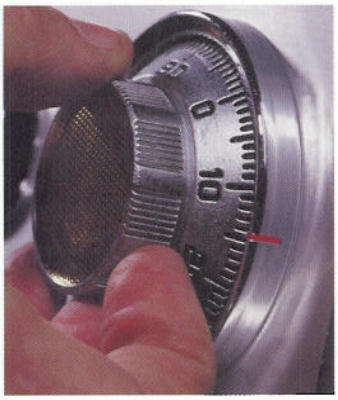
■ The **Lab-in-a-Box** technology was recently licensed to Belhaven Applied Technologies in Kennewick, Wash. Lab-in-a-Box, originally designed for military engines, is an innovative fluid analysis/diagnostics technology that will provide equipment owners valuable information about the condition of engine and drive machinery—while the equipment is in operation.

■ The **Acoustic Inspection Device (AID)** has been licensed to Mehl, Griffin and Bartek. AID uses ultrasound to examine and identify contents of sealed containers. U.S. Customs sponsored this commercialization, but since the terrorist attacks on Sept. 11, interest in homeland security applications is developing rapidly.

■ The **Personal Security Scanner** has been licensed to Safeview of Menlo Park, Calif. The holographic imaging system can identify metallic and nonmetallic objects concealed under clothing, and also has the potential for detecting plastic explosives. X-ray imaging systems subject the body to ionizing radiation; however the holographic imaging system's millimeter-wave scanning technique is harmless. The system was developed for the Federal Aviation Administration to screen airline passengers for weapons.

■ The same **scanning technology**, already commercialized for security scanning, is being readied for custom-fit apparel applications. The scanner would allow consumers the ability to store their body measurements in the computer and to use designer software to "virtually" tailor and try on designer clothes in the convenience of their own homes.

■ **Radio Frequency Tag** technology was licensed in 2000 to a spin-off company, Wave ID, which was created to develop and sell Radio Frequency (RF) Identification systems. RF tags are wireless communication devices that have exceptionally long range, vary in size, and can be designed to identify and locate or monitor items for inventory and asset tracking. Within a year, Wave ID was purchased by Alien Technology, a high-tech electronics manufacturing company based in the Silicon Valley.



■ **Secure Safe**, also known as Smart Safe, is designed to ensure that safes, security containers or any locked cabinets are properly closed and secured prior to the user leaving the room. PNNL is putting this technology to use in its own facilities as well as other U.S. Department of Energy facilities to help prevent human errors when handling classified materials. ●

For more information on these technologies, see **www.pnl.gov/nsd/commercial/**. For a list of technologies available for licensing, go to **http://availabletechnologies.pnl.gov/**.

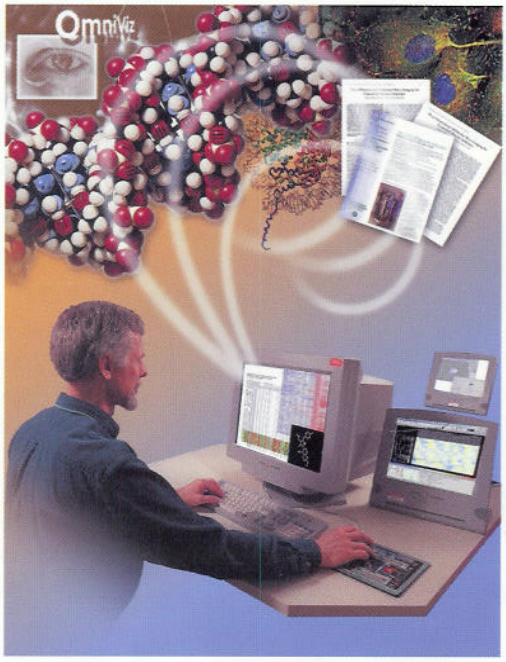
Special thanks to contributing writer, Sue Chin

NOTABLE *Achievements*

R&D Magazine recognizes PNNL innovation

Researchers at Pacific Northwest National Laboratory and at OmniViz Inc., a Battelle subsidiary, were recognized by *R&D Magazine* in June for developing one of the 100 most significant innovations of 2001.

The winning technology is a data mining and visualization software tool called OmniViz®, commercialized by OmniViz Inc. OmniViz® products provide visualization and analysis tools that enable scientists, researchers, mathematicians and other business professionals to efficiently and rapidly mine large volumes of data.



The software provides unique analysis capabilities for unstructured text, numerical data, categorical information and genomic sequences by creating an integrated, interactive visual representation of the information content and associations. "OmniViz® lets people analyze all sorts of diverse data and lets them see their results presented as a unified visualization on a single computer screen," said Gus Calapristi, one of the PNNL researchers involved with the project.

Because the OmniViz® visualization tools enable scientists and business professionals to integrate analyses across multiple data types and across domains, researchers are predicting increased productivity, decreased time to market and reduced business risks for their customers.

Scientists working in the life sciences are particularly interested in OmniViz® software because it can handle the growing volume of diverse types of information inherent in biological research and development. For example, the software's unified visualization techniques enable users to see the linkages between data from gene chip experiments, data from research papers and related protein sequences. Besides finding known linkages, OmniViz® visualization and inspection tools can uncover new relationships between data types that were neither specified nor suspected by the user.

The R&D 100 Award competition is conducted annually by *R&D Magazine* to honor the most promising new products, processes, materials or software developed throughout the world. Awards are based on technical significance, uniqueness and usefulness. PNNL has received 59 R&D 100 Awards since 1969, including 52 since 1988. ●

■ **www.pnl.gov/news/2002/02-17.htm**
■ **www.omniviz.com**

Policy analyst elected to American Academy of Diplomacy

Richard Benedick and his work have been recognized in a way that demonstrates the significance of the environment and science fields in foreign policy. In July, the global change policy analyst from Pacific Northwest National Laboratory became the only person elected to the American Academy of Diplomacy whose role has stretched beyond more traditional foreign policy.

The academy is an association of 100 former cabinet secretaries, ambassadors and statesmen who have made considerable contributions to American foreign policy. Benedick's contributions to global environmental affairs include

■ serving as chief U.S. negotiator and a principal architect of the historic Montreal Protocol on protection of the Earth's ozone layer

■ authoring the award-winning book *Ozone Diplomacy*

■ serving as Deputy Assistant Secretary of State for Environment, Health and Natural Resources, supervising policy formation and international negotiations

■ leading policy divisions at the U.S. State Department.

Benedick currently is based at the Joint Global Change Research Institute in College Park, Md., a partnership between the University of Maryland and PNNL. ●

PNNL bringing genomes to life

Through the U.S. Department of Energy's Genomes to Life program, Pacific Northwest National Laboratory will receive $10.6 million over three years to develop tools to analyze the network of protein complexes within cells. The funding is part of $23.4 million awarded as a result of a joint proposal led by Oak Ridge National Laboratory (ORNL).

The two national laboratories will develop next-generation technologies for isolating, identifying and characterizing groups of proteins, known as protein complexes, within microbial cells.

"The DNA sequence provides instructions to an organism, telling it what proteins to create," said Steve Wiley, the PNNL leader for the project. "By learning about those protein complexes—which may number in the thousands and change constantly—we will take another step toward understanding the molecular processes that allow a cell or organism to function."

The project's ultimate goal is to understand cells and their components in enough detail to predict, test and understand how biological systems respond to changes in their environment.

Scientists will investigate protein complexes in two microbes known for qualities that potentially could be harnessed for environmental solutions. *Shewanella oneidensis* can transform metals and toxic materials into harmless forms and *Rhodopseudomonas palustris* plays a significant role in the Earth's carbon cycle.

Researchers will identify the protein complexes in these microbes as well as how they function and interact. They also will learn about the changes in protein complexes that occur in response to external stimuli.

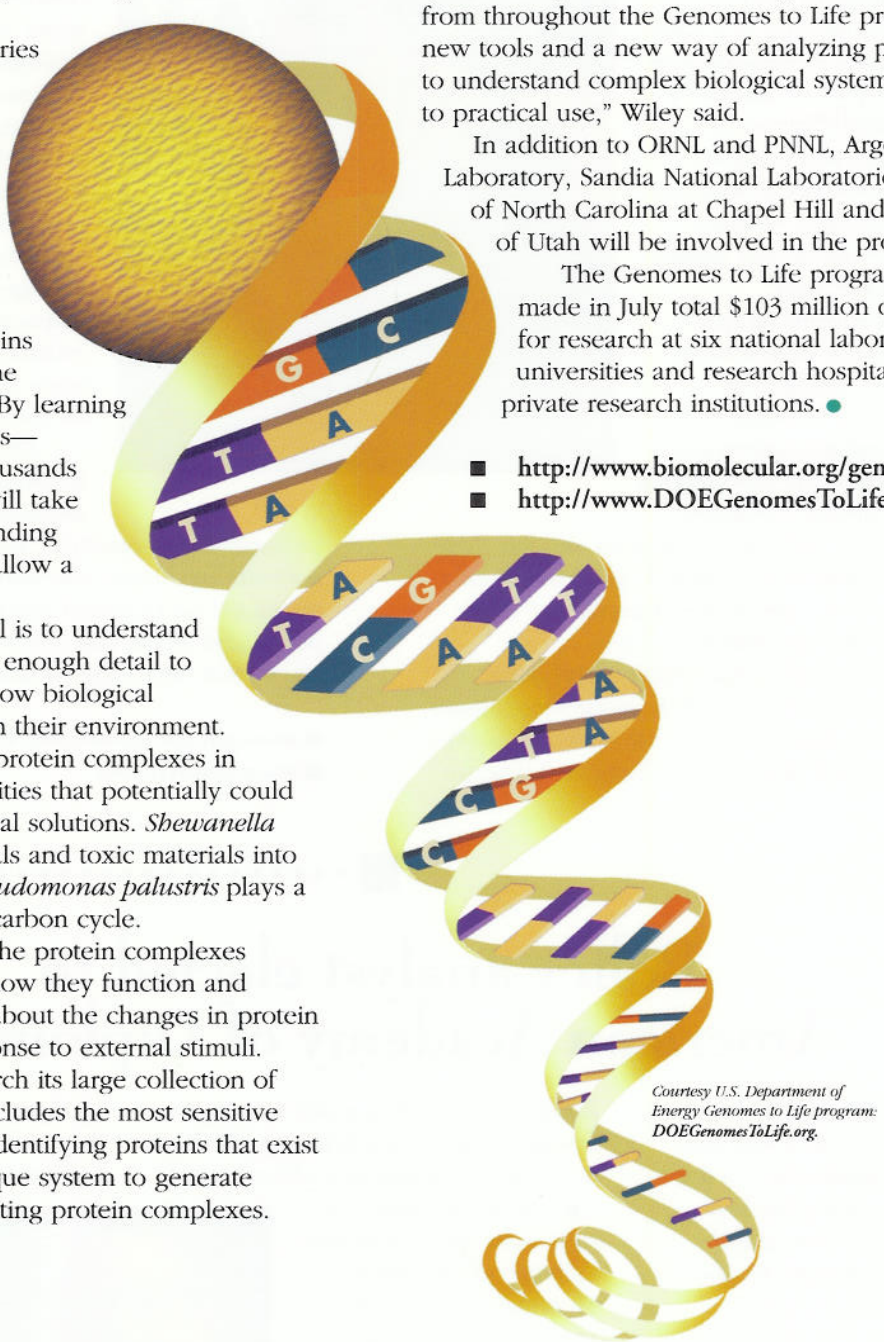
PNNL brings to this research its large collection of mass spectrometers, which includes the most sensitive and rapid tools available for identifying proteins that exist in small quantities, and a unique system to generate "affinity tags" for quickly isolating protein complexes.

As researchers at PNNL work with the two microbes, they will develop new tools that could be used to automate the protein isolation process, allowing for faster identification of more protein complexes as research progresses. They also will enhance mass spectrometry methods and integrate computational data from throughout the Genomes to Life program. "We need new tools and a new way of analyzing protein function to understand complex biological systems and put them to practical use," Wiley said.

In addition to ORNL and PNNL, Argonne National Laboratory, Sandia National Laboratories, the University of North Carolina at Chapel Hill and the University of Utah will be involved in the project.

The Genomes to Life program awards made in July total $103 million over five years for research at six national laboratories, 16 universities and research hospitals, and four private research institutions. ●

- **http://www.biomolecular.org/genomes/index.html**
- **http://www.DOEGenomesToLife.org/**



*Courtesy U.S. Department of Energy Genomes to Life program: **DOEGenomesToLife.org.***

Homeland Security Initiative ready to roll

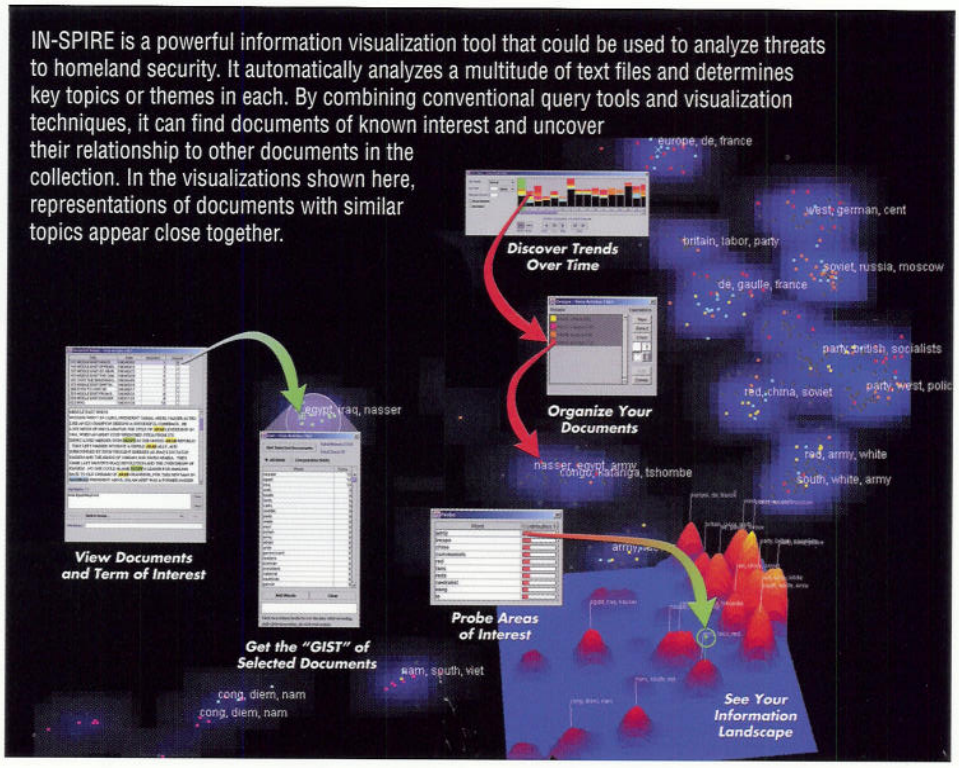
In the year since the terrorist attacks that changed the world, scientists and engineers at Pacific Northwest National Laboratory are continuing on a path begun 40 years earlier—supporting the U.S. government's national security mission.

In addition to a diverse portfolio of technologies related to national security issues, the Laboratory has designed a new Homeland Security Initiative. The initiative will continue to support advances in science and technology, increasing the Laboratory's high-impact contributions to our nation's homeland security.

The initiative focuses efforts on three primary components: dynamic information analysis and decision support, detection and characterization methods, and technology implementation. "We're going from the sensor physics on the front end all the way through analysis and decision support. You have to tackle this problem end to end to make the kind of gains needed to solve a very difficult problem," said Doug Lemon, who leads the initiative.

Dynamic information analysis involves synthesizing information from multiple sources, including documents, sensors, measurements, images, financial figures and the Internet, mathematically computing the signatures for each and comparing them to identify relationships. "So you can see that this financial transaction and this measurement at an airport and the person's face that appears in this box are all part of a plot," Lemon said. Dynamic information analysis not only will pull together all these diverse types of information, but it will be able to process millions of records a day.

PNNL already has technology that can be used in information analysis, such as IN-SPIRE, an information visualization technology offering statistical analysis, and Starlight, an information modeling technology providing spatial and temporal analysis. But the semantic element,



IN-SPIRE is a powerful information visualization tool that could be used to analyze threats to homeland security. It automatically analyzes a multitude of text files and determines key topics or themes in each. By combining conventional query tools and visualization techniques, it can find documents of known interest and uncover their relationship to other documents in the collection. In the visualizations shown here, representations of documents with similar topics appear close together.

how meaning is extracted from words, is still missing. There is currently no one tool that can pull it all together.

Information analysis is only as good as the data provided. As part of the initiative's detection and characterization component, the Laboratory will develop advanced detection and characterization methods, such as analytical separations, sensors and measurement systems to detect chemical, biological, radiological and nuclear materials. These advanced technologies will allow users to collect, concentrate and identify samples in the field faster and less expensively than current technologies, providing higher detection rates, fewer false alarms and faster response.

Finally, the Laboratory will develop methods and technical support that will allow technology users to implement tools quickly and effectively. "The Laboratory is deeply committed to being a technology leader and partner with end-user agencies that deal with all aspects of homeland security, especially those in the Northwest," Lemon said. "We are involved in many applications right now, such as infrastructure protection, and we expect to be involved in many others, such as community-based bio-surveillance and protection as our work expands."

The initiative will be launched in 2003, but in the meantime, PNNL has numerous other technologies applicable to homeland security. These technologies include sensors and electronics for threat detection, state-of-the-art cyber security and information assurance tools, information visualization technologies, atmospheric monitoring and research work, and training for weapons of mass destruction emergency response. Some security-related technologies already have been licensed for commercialization (see story page 12). ●

For Homeland Security Highlights see **www.pnl.gov/news/notes/summer02.htm**

Radiochemical Processing Laboratory plays key role in cleanup

Although not as well known as the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), the Radiochemical Processing Laboratory (RPL) played an important role in bringing EMSL to life in 1997. RPL fulfilled a commitment that Pacific Northwest National Laboratory made to the U.S. Department of Energy to provide a place to conduct the radioactive component of research at EMSL, a national scientific user facility and research organization.

Both are world-class laboratories for their type, and anchors to PNNL's work in researching, developing and deploying solutions to our country's critical environmental problems.

RPL's mission is to create and implement innovative processes for environmental cleanup and the beneficial use of radioactive materials. This includes processes for advancing the cleanup of radiological and hazardous wastes, processing and disposing of nuclear fuels, and producing medical isotopes. The RPL also is the Laboratory's only Hazard Category II nuclear facility and one of only two facilities dedicated to multiprogram nuclear science and engineering research that are fully functioning in the U.S.

"Our expertise lies in development, scale-up and deployment of first-of-a-kind processes to solve environmental problems," said Dale Knutson, who manages PNNL's radiochemical science and engineering program. "RPL really complements the fundamental research EMSL is doing in this area. RPL's capabilities provide the deployment path for the next steps in research using nuclear materials." The RPL staff and facilities are capable of performing any mission that requires radionuclide handling, technology development or process optimization. ●

■ **http://rpl.pnl.gov**

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