Breakthroughs

Science. Technology. Innovation.

WINTER-SPRING 2003

EMSL: The first five years and a blueprint for the future

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PACIFIC NORTHWEST NATIONAL LABORATORY

OPERATED BY BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Breakthroughs

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editor's screen

October 16, 1996. The sun was shining on Pacific Northwest National Laboratory as well-wishers assembled for the dedication of the U.S. Department of Energy's newest user facility, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). The presence of Energy Secretary Hazel O'Leary and other DOE leadership underscored the importance of the ceremony—and the stature of the facility. Although the mood was celebratory, there was a sense of sadness, as the champion and namesake of the new facility, Bill Wiley, was not on hand to help observe the realization of his vision. Wiley had passed away a few months earlier. Still, those attending remember it as a special day. EMSL's potential seemed as bright as the autumn sun.

Approximately one year after the dedication, EMSL became fully operational. In the five years that have followed, many agree that the facility has delivered on its early promise.

As EMSL passes the five-year milestone, we wanted to revisit this unique research facility. In this issue, writer Andrea McMakin provides a fascinating account of EMSL history; we talk with Jean Futrell, EMSL's first permanent director, about the early challenges; and we interview the current director, Bill Rogers, about the path forward, which will be as challenging as the first five years—perhaps more so. We focus on EMSL capabilities, scientific successes and new approaches to research.

Also in this issue, we introduce you to Pacific Northwest National Laboratory's new director, Dr. Leonard Peters, and highlight PNNL's latest laurels, including a fifth consecutive outstanding rating conferred by DOE, and prestigious national recognition for science and technology. ●

Contents

Peters selected as next leader of PNNL

Dr. Leonard K. Peters is the new director of Pacific Northwest National Laboratory, succeeding Dr. Lura Powell.

Peters joins PNNL from Virginia Polytechnic Institute and State University, where he served as Vice Provost for Research.

"I am very excited and proud to join a laboratory of PNNL's great stature," Peters said. "Its top-flight staff and capabilities in fundamental science, applied science, energy, environment and national security are tremendous. And, given the fact that I once worked at the Laboratory on an 18-month assignment, I already have a great appreciation for the Lab and its staff."

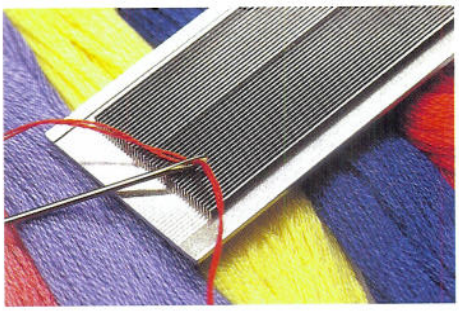
"We believe that Dr. Peters' science and technology credentials, experience in leading diverse research programs and community service record are a great match for the Laboratory and its future direction," said Carl F. Kohrt, president and CEO of Battelle, which operates PNNL for the U.S. Department of Energy's Office of Science.

Dr. Raymond L. Orbach, director of the Office of Science, echoed that sentiment, adding, "Dr. Peters has a strong track record in science and technology and is a proven innovator in research and public-private partnerships. Just as important, he has been nationally recognized for his science and community service innovations at the state and local level."

Peters holds bachelor's, master's and doctorate degrees in chemical engineering from the University of Pittsburgh and spent part of his career as a researcher in atmospheric chemistry. Since 1993, he has managed Virginia Tech's $230 million research program, which ranges in scope from biotechnology and materials to transportation and information technology. ●

Lab, OSU join in new microproducts institute

Pacific Northwest National Laboratory and Oregon State University celebrated a "virtual groundbreaking" in Portland, Ore., recently for their new Microproducts Breakthrough Institute.



The institute will advance the science of microtechnology, provide educational opportunities through OSU and promote regional development by commercializing new products. "We're not working on technologies that are 20 years away from deployment," said Ron Adams, dean of the OSU College of Engineering. "Our goal is to develop breakthrough products that lead to new businesses immediately."

Examples of microtechnologies under development include biosensors as small as lapel pins that could detect chemical and biological warfare agents and other environmental toxins like *E. coli*, and heat-actuated air conditioning units no bigger than a shoebox that would use waste engine heat to cool automobiles.

The institute should help spawn a new industry in the Pacific Northwest based on small, lightweight and more efficient chemical, energy and biological systems for commercial and non-commercial use. Millions of dollars in research, important scientific discoveries, new start-up companies and more jobs for Pacific Northwest residents may soon emerge from this initiative, organizers say. ●

NOTABLE Achievements

Scientists win prestigious awards

Five Pacific Northwest National Laboratory scientists were recognized recently for their career accomplishments. Two of the scientists won prestigious national awards from the American Chemical Society (ACS).

David Dixon received ACS's 2003 Award for Creative Work in Fluorine Chemistry. The award honors Dixon for "advancing the use of computational chemistry to bring unique understanding to the field of fluorine chemistry, especially chlorofluorocarbon replacements, organofluorine molecules and inorganic fluorides."

Richard D. Smith was awarded the 2003 ACS Award in Analytical Chemistry. Smith's accomplishments include developments that integrate two analytical disciplines: separation science and mass spectrometry. Smith's leading role in applying these combined techniques to modern bioanalytical problems and biological systems characterization has led to numerous advances in analytical chemistry.

Also, three PNNL scientists have been promoted to Scientist and Engineer VI, one of the highest levels of scientific achievement and recognition at the Laboratory.

James Cowin has made significant contributions to understanding the chemistry and structure of solid and liquid interfaces. **Peter Martin** is internationally recognized for his thin-film coatings research. **Denis Strachan** has worked to achieve a better understanding of glass and ceramics behavior and interactions with radioactive waste materials, laying the foundation for decisions on waste and safety issues.

There are 48 active Scientist and Engineer VIs, who also serve as members of the Council of Fellows, an advisory group that helps set PNNL's science and technology agenda. ●

Laboratory gains research grants

Pacific Northwest National Laboratory came out a winner in two separate U.S. Department of Energy research grant competitions recently.

The Laboratory was awarded $5.2 million to fund research aimed at resolving some of the nation's most challenging environmental cleanup issues. The awards are part of the DOE Environmental Management Science Program (EMSP) and are much sought after by national labs and universities. PNNL is involved in 24 percent of this year's EMSP projects.

Most of the Laboratory's awards are targeted at research involving residual contaminants in groundwater and subsurface soil. PNNL scientists believe this work will help them understand how chemical and radioactive contaminants behave in groundwater and subsurface soil, and is likely to provide the scientific basis for a final remedy to some of Hanford's groundwater plumes and other contaminated sites.

The Laboratory also won three Nuclear Energy Research Initiative (NERI) awards, worth a total of $1.3 million per year over three years. More than 197 proposals, submitted by scientists at national laboratories, universities and industry, were considered in a rigorous peer review process to arrive at the final 24 funded projects.

Research on two of the NERI awards will seek better understanding of the structural behavior of materials needed to meet new, longer-life requirements for materials in the U.S. nuclear reactor fleet. The third award focuses on automating quality assurance techniques for the fuel systems of advanced gas-cooled reactors. This work is crucial to the safety of new high temperature reactors suitable for producing both electricity and hydrogen for future transportation needs. ●

DOE confers fifth "Outstanding" rating

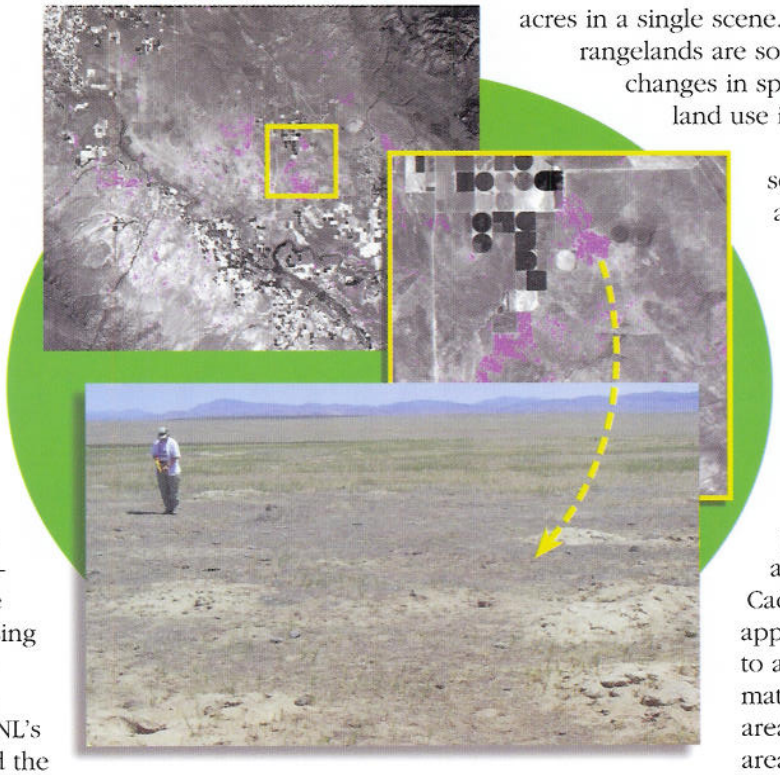
The U.S. Department of Energy has awarded Battelle, operator of Pacific Northwest National Laboratory, an Outstanding rating for performance in fiscal year 2002. Outstanding is the highest designation bestowed by DOE. Battelle has achieved the rating annually at PNNL since 1998.

Although DOE called for improvements in PNNL's practices related to work authorization and funding, DOE Richland Operations Office Manager Keith Klein indicated the agency continues to be satisfied with Battelle's overall performance in managing PNNL and is particularly pleased with progress in science, operations and safety. ●

Technology on the range

Ranchers, farmers, loggers and recreationalists throughout the West are being asked to share rangelands. With more groups using Western rangelands, it has become increasingly important to monitor the land to maintain it and to guard against overuse.

The Bureau of Land Management has been tasked by Congress with reporting the conditions and changes on the land it manages—all 262 million acres of it. Pacific Northwest National Laboratory researchers have developed a unique way of applying remote sensing capabilities to monitor these rangelands. "It sounds like a cliché, but it's true," said PNNL's Larry Cadwell, who managed the project. "We were challenged to do it better, faster and cheaper."



The BLM asked PNNL to find a cost-effective and easy-to-use way to sample BLM lands, locating areas of management concern such as bare soil. Remote sensing tools, including low-level aerial photography and digital imagery from satellites, were the logical choice for cost-effective monitoring.

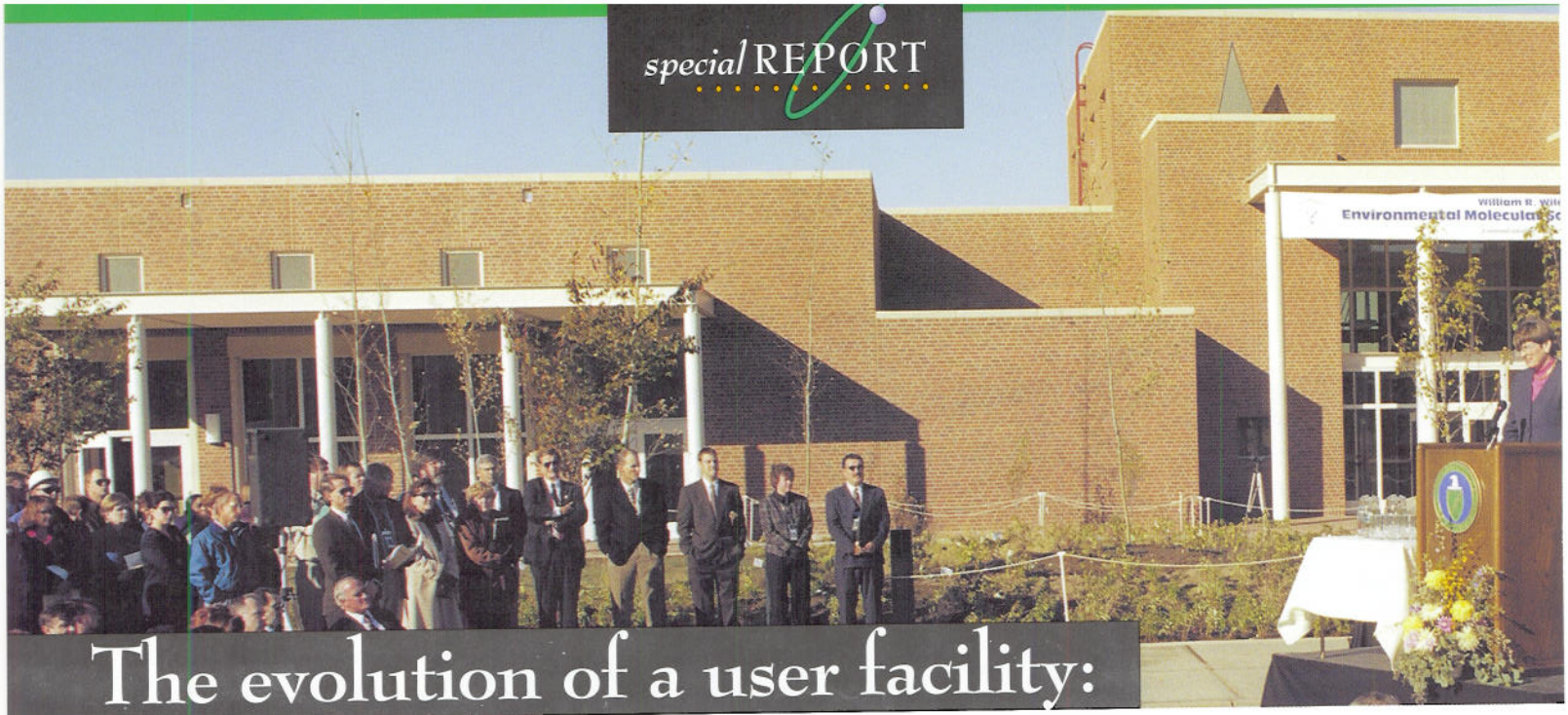
"Each pixel of a remote sensing image gives a spectral signature for that area on the ground, and when you have a change in vegetation cover resulting from some disturbance, that change is reflected in the spectral signature," Cadwell said. Finding where the spectral signature differs from the expected or normal pattern of the site helps identify areas of overgrazing, weed invasion or fire damage.

Researchers considered using Landsat satellite imagery because it's fast and can capture eight million acres in a single scene. But eight million acres of rangelands are so diverse that isolating small changes in spectral signature related to land use is nearly impossible.

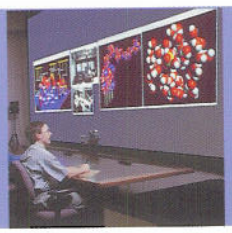
So using available soil and vegetation data, analysts stratified the imagery by dividing the landscape into similar areas according to soil type, vegetation and slope. "Once we have homogenous areas and look at the spectral data for those individual areas, it's much easier to detect a change or abnormal condition," Cadwell said. PNNL analysts applied statistical techniques to analyze the spectral information from homogenous areas to detect anomalous areas or "hot spots."

Analysts envision the ultimate product as a web-based system where BLM land managers and ranchers could view maps of land conditions and areas of concern. By entering location data, they could pinpoint extreme amounts of vegetation cover or exposed soils. Over time, users will see trends, such as more invasive weeds or increased soil erosion.

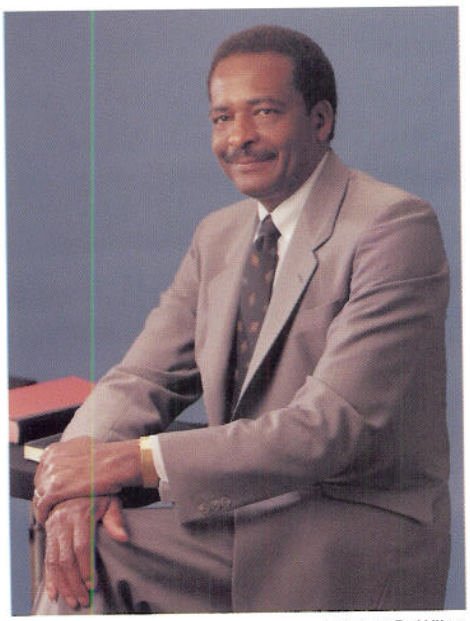
PNNL is using these techniques to help the BLM manage fuel accumulations in the dry rangelands of southern Idaho. In arid and semi-arid regions, vegetation is less dense and often dormant through the summer and fall. Vegetation maps derived from satellite imagery may be inaccurate because the spectral response mainly reflects soils. PNNL's methods for detecting subtle differences in spectral responses allow better mapping of salt desert and shrub-steppe vegetation for fuels analyses. ●



The evolution of a user facility: VISIONS AND



EMSL pioneers reflect as facility celebrates five-year anniversary



William R. Wiley

The evolution of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is like the growth of a much-loved child. Like a precious newborn, EMSL was much anticipated, carefully prepared for and underwent some hard labor to enter the world. Now in the maturity of its fifth year, EMSL is fulfilling many of the dreams envisioned by its "parents"—while showing promise of even greater achievements.

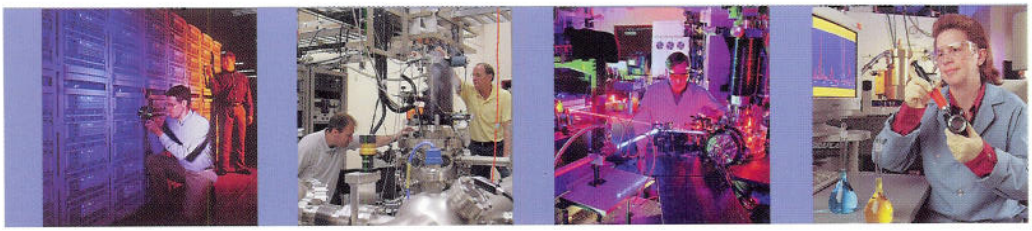
As a national scientific user facility in Richland, Wash., EMSL is operated by Pacific Northwest National Laboratory for the U.S. Department of Energy's Office of Biological and Environmental Research. The 200,000-square-foot facility houses advanced experimental and computational tools for scientists engaged in fundamental research on the physical, chemical and biological processes that underpin critical scientific issues. With its collection of 100 pieces of major research instrumentation, including some of the world's most powerful analytical tools, EMSL is unparalleled in the breadth and quality of science capabilities under one roof.

Bill Wiley's vision

EMSL opened for business in October 1997, but the concept was set in motion a decade earlier. A 1986 report by the National Academy of Sciences galvanized PNNL Director William Wiley's vision for the facility that eventually became EMSL. The report identified a number of scientific challenges that could be solved only through fundamental research—exploration that reveals a new understanding of the natural world.

Wiley argued that complex problems in environmental cleanup, energy efficiency and health had to be solved at the molecular level. He envisioned a center that would address these challenges by bringing together theoreticians with expertise in computer modeling of molecular processes and experimentalists from the physical and life sciences.

DREAMS



At that time, the concept of an integrated suite of capabilities in one place represented a dramatic departure from DOE's existing user facilities, which typically housed single large pieces of equipment that did one thing really well. But Wiley envisioned a user facility that was integrated and collaborative: "In the past, we tried to put nature in academic boxes. We must now expand our vision, so that the reality is consistent with the truth of the universe, the environment and the humans in it. Problems don't come in small, unique, compartmentalized packages. We must recognize the interrelationships."

Selling the concept

Wiley assembled a team to flesh out his concept and begin building advocacy in the scientific, academic and political communities. To add credibility to the concept, Wiley set up a prototype center, complete with 60 staff and advanced equipment already at hand, in an existing building at PNNL. Battelle, which operates PNNL, invested $8.5 million over four years in people, equipment and facilities for what was then called the Molecular Science Research Center.

Teams began writing proposals to demonstrate the scientific quality necessary to justify DOE's capital investment in such a facility and its equipment. Center interim director Adrian Roberts began traveling with his team around the Pacific Northwest, promoting the concept to university and community leaders while seeking input about the nature of the scientific work to be conducted there.

The reaction to the proposed new facility ranged from "incredulous to supportive," Roberts recalls. Some university leaders saw it as potential competition. DOE assembled teams of nationally eminent scientists who scrutinized the early ideas in review after review. Gradually, support grew.

Roberts remembers those pioneering days as challenging but exciting, with Wiley always urging them on through the obstacles. "He saw the dream; there was no stopping him. He wouldn't take no for an answer, and that energized

"Over a decade ago the Office of Science and PNNL embarked on an experiment—to build a facility to conduct science at the molecular scale. There was not much of a roadmap, just dedicated people with a dream. Five years ago that dream opened with this unique facility. The distinctive collection of creative scientists and users, one-of-a-kind instruments, and computational capability in EMSL has made the experiment a success. EMSL has produced cutting-edge science, important not only to the environment, but also to biology, chemical physics and computational chemistry. Now EMSL is about to embark on another experiment— a new approach that will bring a community of users together around the full set of EMSL capabilities to solve a major scientific question. I look forward to future EMSL discoveries and innovative approaches to the molecular sciences."

Ari Patrinos
Associate Director for Biological and Environmental Research
DOE Office of Science

"The EMSL, as a user facility, has given researchers across the country access to state-of-the-art instrumentation and the superb professionals who manage it. In my own research, the extraordinary capabilities of the High-Performance Computing Center allowed us to address problems in the electronic structure of heavy-element systems that we could not even fathom prior to that. The new capabilities of the upgraded HPCC will provide yet another quantum leap for quantum chemistry!"

Bruce Bursten
Distinguished University Professor and Department Chair
Department of Chemistry
Ohio State University

"The Environmental Molecular Sciences Laboratory is a world-class research facility for the advancement of science and technology. Scientists from the U.S. and around the world are able to use this laboratory to perform vital research on pressing environmental and human health issues."

Gary Locke
Governor
State of Washington

"The EMSL's unique mass spectrometry instrumentation, advanced computational and instrumentation development capabilities have allowed our research to study biological processes in a way that has not been possible previously. A result has been our ability to examine essentially all of an organism's proteins in one measurement and provide a basis for truly understanding how complex biological systems work."

Richard D. Smith
Battelle Fellow and
Chief Scientist
Fundamental Science Directorate
PNNL

"Five years ago I had the pleasure of being part of the EMSL when this unique facility opened its doors. The EMSL scientists, scientific users, and the facility capabilities remain at the leading edge of molecular research five years later. I look forward to working once again with my former colleagues to ensure that EMSL remains a premier national user facility for many years to come."

Teresa Fryberger*
Director
Environmental Remediation
Sciences Division
DOE Office of Biological and
Environmental Research

*Served as interim director of EMSL, 1997–99

us," Roberts said. "Everyone on the team felt they were engaged in a disruptive activity that would change the face of the Lab and science itself."

In 1988, the effort rose to a new level when several highly regarded scientists were recruited to lead the science programs and attract other premier staff. Charles Duke, Mike Knotek, Thomas Dunning and Steve Colson were among those lured away from prestigious positions in industry, Ivy League research universities and other national labs. They were attracted by the opportunity to create an astounding collection of advanced instruments and science programs and to collaborate in ways not possible in their current positions. For the next five years, they launched more than 100 technical workshops across the country to hammer out the details of the necessary research and instrumentation. They also recruited more staff and formed an independent advisory panel.

As the concept solidified and gained visibility, it also became a target. Some environmental cleanup contractors didn't want to hear that science was needed to solve remediation problems, Mike Knotek said. Some business leaders were worried that a cleanup process accelerated by science would reduce the flow of government dollars to their communities. Some Congressional representatives wanted to site EMSL in their own districts, while others tried to kill it. "For roughly six years, this thing was in the ditch every two weeks and we had to get it out," Knotek said.

Finally in 1993, DOE authorized construction of EMSL at a cost of $230 million. The original multi-story design had since given way to a long, low design with 80 individual labs, sited on bedrock for stabilization. Each lab was electronically, seismically and thermally controlled to house the highly sensitive instruments inside.

After an initial groundbreaking at a site near the Columbia River turned up some Native American bones, the site was moved farther inland near existing buildings at PNNL. The facility was dedicated in Bill Wiley's honor in October 1996, a few months after he unexpectedly passed away. Construction was completed in August 1997, and the EMSL opened for full operations as DOE's newest national scientific user facility on Oct. 1, 1997.

Jean Futrell reflects on his EMSL

In 1998, Jean Futrell was leading a relatively comfortable life. He held an endowed professorship at the University of Delaware and was internationally recognized for his contributions to mass spectrometry. Little did he know that a daunting challenge was on the horizon—at the William R. Wiley Environmental Molecular Sciences Laboratory.

EMSL was seeking a permanent director. Futrell was familiar with the facility, having participated in the early planning. He also was familiar with—and committed to—the philosophy that EMSL champion Bill Wiley had used in pursuing the facility. That approach, Futrell says, was grounded in a national report, *Opportunities in Chemistry*. Futrell had used the report findings as a template for leading the University of Delaware's drive for excellence in chemistry and biochemistry.

After EMSL became reality, Futrell was contacted by a search committee looking for director candidates. He discussed the job with his wife, Anne Graham, an art professor at the University of Delaware. Although the move to Richland would be life changing for both of them, they decided that Jean would pursue the new opportunity.

"As a participant in the workshops that planned EMSL and a member of the facility's Scientific Advisory Board, I was very aware of EMSL's extraordinary capabilities and staff," he said.

Futrell was selected to lead the facility in the fall of 1998, and he began working full time in the position in February 1999. "It was important that the first director be a practicing scientist as well as a manager," he said. "Leading by example and understanding the frustrations posed by bureaucracy while conducting world class science helped me build rapport with the scientific staff."

EMSL today

EMSL has an annual research budget of $30 million and another $36 million for operations. DOE supports the lion's share of EMSL research, but funding from partners such as the National Institutes of Health is increasing. There's a growing emphasis in biology, such as studies on using naturally occurring microbes for environmental cleanup, alternative energy and carbon dioxide reduction in the atmosphere.

More than 100 onsite staff plus about 1,700 national and international users annually draw on EMSL for everything from understanding environmental phenomena to creating new materials. Scientists are lined up to use one of the world's largest high-performance nuclear magnetic resonance spectrometers for chemical, biological and materials research. Others are anticipating access to the Linux-based supercomputer. When fully installed in 2003, the 11.4-teraflop system will be used to answer questions such as how proteins interact in a living cell. And EMSL continues to offer state-of-the-art mass spectrometry capabilities with its impressive collection of instruments, including an 11.5-tesla magnetic field Fourier transform ion cyclotron resonance mass spectrometer.

Consistent with DOE's mission to help the scientific community, EMSL users are not charged a fee for research using EMSL resources if the results are published in open literature. Users who want to keep their research findings to themselves, such as industry representatives developing a proprietary product, must pay a fee to help recover taxpayer-funded equipment costs.

Recent benchmarking studies with other national user facilities showed that EMSL service to its users is best in class, according to EMSL Associate Director Allison Campbell. "We really cater to our users, giving them as much or as little help as they want," she said. An early example was converting unwieldy three-day training procedures for EMSL users into a web-based program that now takes only one or two hours and can be completed almost all in advance. "Now when they get here, their time doing science is maximized," Campbell said.

In fact, EMSL has paved the way for DOE's next-generation user facilities, according to Reinhold Mann, PNNL's chief research officer. "I get a lot of inquiries

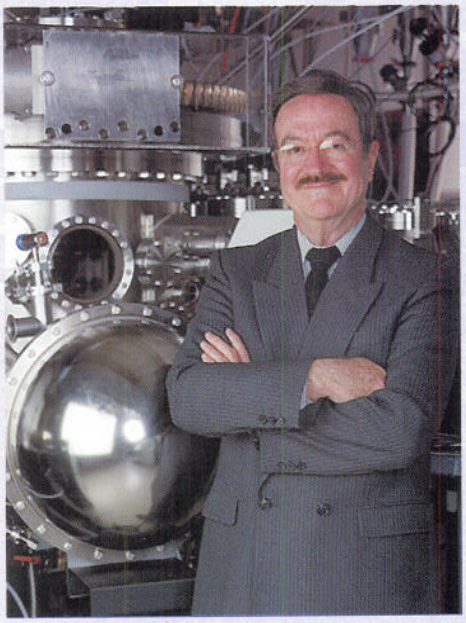
"EMSL offers scientists the unique opportunity for research at the interface between physical, chemical and computer sciences. Significant research has been accomplished at EMSL, and I anticipate even greater accomplishments as PNNL's strength grows in its systems biology program and new research tools, such as the 900-megahertz NMR magnet and the new supercomputer, are put into use."

Paul Kruger
Associate Manager for Science and Technology
DOE Richland Operations Office

"Access to the Molecular Science Computing Facility resources—the unique massively parallel computers and the impressively capable Molecular Science Software Suite with NWChem—has enabled us to study the structures and spectral properties of complexes containing actinides like uranium at unprecedented levels of accuracy, providing unique information about these highly reactive and radioactive molecules."

David A. Dixon
Battelle Fellow
Fundamental Science Directorate
PNNL

experience



Futrell headed a management team composed of associate directors who also served as research leaders and deputy directors who shared the administrative work load. A capable group of office staff interfaced with users and facilitated EMSL operations.

Teresa Fryberger, EMSL's interim director from October 1997 to February 1999, was both Futrell's senior deputy and an "invaluable bridge to EMSL's immediate past, as well as to PNNL and to DOE," he noted. Interestingly, EMSL now reports to Fryberger, who heads DOE's Environmental Remediation Sciences Division.

Futrell felt strongly that a key element of his job involved serving as EMSL's external champion—working to raise the visibility of the research facility with DOE Headquarters, potential users and other agencies. He also believed it was imperative to continually enhance EMSL's scientific attributes. He avidly supported strengthening the facility's mass spectrometry capabilities for proteomics-related research. And he worked to obtain two powerful new research tools that arrived in 2002, a 900-megahertz nuclear magnetic resonance spectrometer and a $24.5 million supercomputer. "The hardest one to achieve was the supercomputer. We had to overcome many obstacles. But EMSL must be at the cutting edge of research, so obtaining the computer was very important," he noted. "I always sought to take EMSL's capabilities to the next plateau of what's possible in science."

Futrell left the directorship last year to head up PNNL's Council of Fellows, a select group of researchers who serve as role models and mentors to other research staff and help guide and maintain the direction of PNNL's scientific research. But he carefully tracks and will always be interested in EMSL's progress.

"One of the challenges as EMSL goes forward will be maintaining its broad and unique capabilities. In terms of what can be done in molecular sciences and related areas, EMSL is like having 10 of the best universities rolled into one." ●

"EMSL has established itself as a world leader for the science of metal-oxide surfaces both in terms of the state-of-the-art facilities that were developed for carrying out this science, as well as the expertise that is now resident in the facility. EMSL research, carried out by staff and numerous external users from academia, industry and government labs, has provided major advances in this scientific field. It has been the highlight of my research career to have been a part of this scientific revolution, especially considering the wide-ranging practical benefits that will result from the work."

Charles Peden
Laboratory Fellow
Fundamental Science Directorate
PNNL

"The EMSL construction project provided us the opportunity to design and construct a suite of instrumentation for studying the dynamics and kinetics of surface processes using molecular beams. Using this state-of-the-art instrumentation, my colleagues and I have made important discoveries in such diverse areas as nanoscale amorphous materials, supercooled liquids, astrophysical ices and nanoporous catalytic materials. We have only begun to scratch the surface of the chemistry and physics that can be explored with these instruments."

Bruce Kay
Laboratory Fellow
Fundamental Science Directorate
PNNL

"When I think of EMSL, I think of PNNL visionaries who transformed a vision into a reality; I think of a world-class research facility that has unmatchable batteries of instrumentation; and I think of the unique career opportunities that enable young people to make important contributions to science and technology. I was extremely fortunate to start my career at the birth of EMSL. EMSL allowed me to dream about the most exciting science I could do, and to focus my energy to carry it out. I will always treasure my experience at EMSL."

XiaoLiang Sunney Xie
Professor
Harvard University

from colleagues wanting to know how we manage this heterogeneous set of capabilities under one roof, how we strike a balance for internal and external collaborators' time on machines," he said. The new user facilities DOE is now building at other laboratories, such as nanoscience centers, are going to look and operate very much like EMSL does now, he said.

Hallmark science and tools

Where is EMSL in its life cycle? EMSL Director Bill Rogers said it's past the growth stage, "when we were building programs and attracting people." Now, he said, it's moving into the maturity stage, "where we're coordinating efforts to do more high-impact science."

One gem is the cellular observatory, where scientists study how live cells respond to environmental contamination or other insults including chemotherapy and radiation. Another is the study of protein clusters, using novel, high-throughput mass spectroscopy instruments that were developed at EMSL and then improved further in collaboration with commercial instrument manufacturers.

Using advanced computational and analytical resources, EMSL scientists have identified biotoxins in environmental samples and created a virtual model of the lung. In collaboration with Motorola, EMSL scientists created novel materials and gained new scientific insights that are helping shape next-generation semiconductor technology.

New science tools open doors to new science discoveries. For example, EMSL computer scientists developed software for computational chemistry that won numerous awards and is used worldwide to model subsurface and molecular-level interactions. EMSL has its own Instrument Development Laboratory, where discoveries are benefiting science and industry worldwide. Commercial companies have licensed EMSL-developed innovations such as new mass spectrometers and instruments designed to detect yellow fever.

In fact, scientific and instrument innovations at EMSL have produced more than 60 patents and at least a dozen national awards for scientific merit and technology transfer. EMSL discoveries have been featured on the covers of more than 10 peer-reviewed science journals of international stature.

Full circle

What's ahead for EMSL? EMSL Director Bill Rogers is eyeing ways to further enhance the impact of science done at EMSL, specifically targeting high-profile users to work together on "scientific grand challenges." Rogers also aims to broaden EMSL's funding base while continuing science that can be applied to DOE's mission areas. A high priority is maintaining and upgrading the extraordinary research tools and developing next-generation capabilities for users.

Bill Wiley passed away before EMSL opened for business. Adrian Roberts, who worked with him so closely at the start, has no doubt Wiley would be pleased if he could see EMSL in full operation today. "He would say, that's exactly what I thought it would be—a one-stop shop for science, in an interdisciplinary environment," Roberts said.

Allison Campbell said Bill Wiley's daughter Johari was in awe when she toured EMSL recently after living out of state for several years. "She said her dad would have been immensely proud that his vision was achieved." ●

For more information about EMSL, visit **http://www.emsl.pnl.gov**.

Collaboration at EMSL produces innovative mass spectrometer

The future of proteomics is in good hands with one of the most powerful and versatile mass spectrometers being developed by scientists and engineers from the William R. Wiley Environmental Molecular Sciences Laboratory.

The high-throughput Fourier transform ion cyclotron resonance (FTICR) mass spectrometer and automated liquid chromatography (LC) system is a breakthrough in mass spectrometry capable of improving the understanding of protein production, function and interactions at the cellular level and beyond.

Proteomics is the study of proteins in the human genome that are made and change within a cell over time as the cells respond to disease or changes in their surrounding environment.

"The success of the high-throughput FTICR mass spectrometer and the automation system heralds the next generation of proteomics research," said Harold Udseth, technical leader of EMSL's High Performance Mass Spectrometry Facility.

Mass spectrometers are used to weigh atoms and molecules. This can be done with a precision of one part in five million, which, when applied to the human cell, will enable scientists to learn a great deal about how the cell works. "And once scientists fully understand how human cells work, they can begin to work on methodically solving problems involving things that go wrong in a cell such as cancer," Udseth said.

"The signature of the newest, high-throughput FTICR is the high resolution and high mass measurement accuracy of the system," Udseth continued. "It does better than other mass spectrometers available in measuring the mass of peptides (small structural units obtained by cutting proteins into pieces). It offers such sensitivity and precision that scientists can detect hundreds of thousands of peptide species in a single analysis." Identifying peptides is an important part of proteomics research to determine the role that proteins play in cells and living systems. Researchers expect that more than a million peptides are available in the proteins expressed within human cells.

The mass spectrometer project took nine months of concerted effort by a diverse team composed of scientists from the High Performance Mass Spectrometry Facility and engineers at the EMSL Instrument Development Laboratory (IDL), both of whom brought diverse talent and experience to the table. "It's essential to get the right people in the right place, people who have a desire to work together for a common goal," Udseth said. "In this case, everyone was inspired by the work."

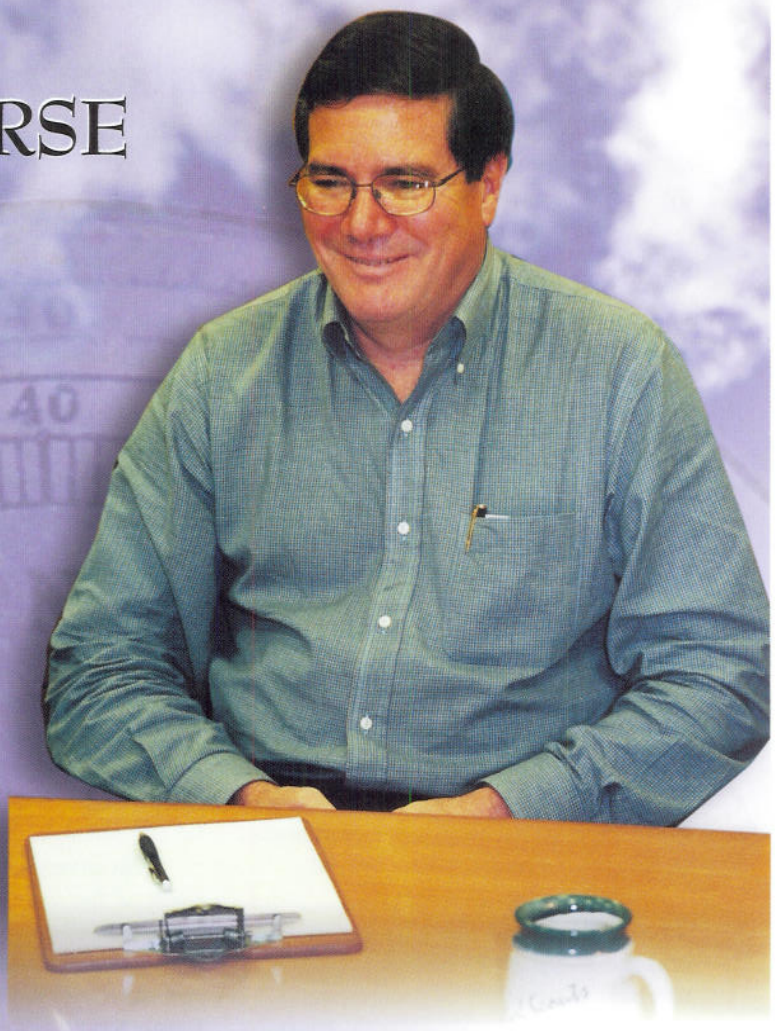
The project required the replacement of the instrument's commercial ion manipulation optics with EMSL's patented ion funnel technology, as well as the design, development and construction of an automated LC system that incorporates a commercial autosampler and PNNL's high-pressure LC technology. Software written by researchers at EMSL is used to control the LC system and integrate it into a single operating system.

"We worked closely with Harold and his staff to understand and provide technical support to overcome the unique challenges of developing this cutting-edge research equipment," said Gordon Anderson, manager of the IDL. The IDL is an integral part of EMSL and includes staff with expertise in electronic circuit design and fabrication as well as software development. "Finding that common, underlying language between scientists and engineers paved the way to a satisfying collaboration," Anderson said. ●

For more information about the FTICR and other mass spectrometers at EMSL, visit **http://www.emsl.pnl.gov**. For more information about the Instrument Development Laboratory, see **http://www.emsl.pnl.gov:2080/docs/idl/home.html**.

A multidisciplinary team composed of scientists and engineers was key to the successful development of the cutting-edge, high-throughput Fourier transform ion cyclotron resonance (FTICR) mass spectrometer. The research tool significantly accelerates proteome analysis and provides accuracy and depth never before reached in proteome studies. This ability greatly enhances the understanding of protein production, function and interactions at the cellular level.

Charting a Course
of growth and success



The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) has experienced a number of successes since it began operations, but EMSL management will not have the luxury of resting on the facility's past accomplishments. The U.S. Department of Energy's Office of Biological and Environmental Research (BER), which oversees EMSL, has high expectations for the facility, particularly related to increasing the impact of the science produced there.

In recent months, EMSL has been reorganized with an emphasis on strengthening the user aspects of the facility. One of the new features is Collaborative Access Teams. These teams of PNNL staff and external users organized around six of EMSL's core capabilities will pursue broad areas of scientific inquiry and support a new research approach referred to as "scientific grand challenges."

Recently we spoke with Bill Rogers, who joined Pacific Northwest National Laboratory in 1999 and was named EMSL Director in July 2002. Rogers is leading what might be considered EMSL's second phase of growth. He recognizes the challenges of taking EMSL to the next level and knows the next five years represent a critical period in EMSL's development and evolution. In our interview, he discusses the identity and strengths of the facility, the path forward and the focus on scientific grand challenges.

If you had to give a description of EMSL to a person who is unfamiliar with this facility, how would you describe it?

Let me share with you *my* first impression of EMSL, not from the perspective of a lay person, but as a practicing scientist. When I set foot in EMSL, I felt like I was in a candy store for chemists. It is a beautiful facility with a beautiful physical plant. EMSL offers a little bit of everything in the way of research instrumentation, and *a lot* in certain areas, which gives researchers the opportunity to do things they can't do anywhere else. In seeking answers to their questions, researchers who come here will find that they have not just one instrument to use but maybe five or more different capabilities. EMSL offers unique research opportunities and it is an outstanding facility by any measure.

Would you describe EMSL's first five years as successful?

I believe EMSL has been a huge success. We have gone through the growth stage, and I think it has been handled very well. EMSL was truly a new laboratory built from the ground up. Bill Wiley (the former Pacific Northwest National Laboratory director and EMSL namesake) recognized that in order for PNNL to prosper in the future, we must build a strong science and technology base. The vision for EMSL was his way of doing that. When Thom Dunning and Steve Colson (early proponents for the facility) were initially given the resources to start significant programs that led to EMSL, the Department of Energy told PNNL that the money could not be used for "business as usual"—that EMSL must be a new type of user facility, with new approaches and new researchers operating it. I think we have been successful in meeting DOE's expectations. Over a five-year time period, we've had 5,500 users, 1,100 technical publications, and 2,000 user projects, representing scientists from every state. Six percent of the users are

from overseas. Right now we are full, and most of our major capabilities are oversubscribed. We can't support many new users. I would say we are through with the growth stage, and growth stage was spectacular. You've heard of the movie where they say "build it and they will come," and here at EMSL, we built it, invited users, and they did come.

With the growth stage now complete, what is EMSL's next phase?

It's going to be very different in the next five years. We are going to be targeting groups of users. In the past, we have seen a lot of single users who come to use one instrument. We want to see more groups of users harnessing major chunks of our research capabilities. We will be starting a new program focused on scientific grand challenges.

What is a scientific grand challenge?

The idea is to bring teams of users—the best scientists in the world, who will not be using a fraction of EMSL's capabilities, but the entire EMSL. The teams would be focused on finding answers to major science questions. An example of a grand challenge focus might be cell signaling—how cells interact with each other and their environment. Who would come? Who would be the users? We envision that the 10 best cell signaling experts in the world would participate.

How would you persuade these pre-eminent experts to come to EMSL?

We hope to make such a compelling argument and show that we have the right capabilities to answer challenging science questions that these folks will have no choice but to sign up or be left behind. This is sort of an experiment in that sense, as this has not been done elsewhere. I think the closest thing you could point to was the Human Genome Project, which was very well defined with a goal of sequencing every base pair. This fiscal year, we will be laying the groundwork for three grand challenges, in biology, subsurface science and likely in the area of catalysis and emissions science. Will we see progress? Absolutely. It's part of our performance evaluation with DOE. Work is currently under way, and by the end of the fiscal year we hope to launch the first two grand challenges.

EMSL appears to be proving itself as a research facility that contributes not just to fundamental science, but across DOE mission areas. Is there a possibility that EMSL can play a major role in issues like global climate change, where there are multiple research needs?

I believe EMSL can play a pivotal role in global climate change research, which is important to BER. We already have a strong presence in this research area. PNNL manages DOE's Atmospheric Radiation Measurement Program, which is external to EMSL. We are involved with the University of Maryland with the Joint Global Change Research Institute. We have outstanding climate modelers at PNNL who are using EMSL's computing resources. We have access to a Battelle-owned atmospheric research aircraft, and, in fact, some of the instrumentation on that aircraft belongs to EMSL. Within EMSL, we have strengths in atmospheric chemistry, and we recently made a strategic hire in this area to further enhance our capabilities. Factoring in all of these resources, I believe EMSL will play a significant role in providing science solutions to the global climate change issue. I mentioned three grand challenges that are planned. Two others are in the works—one is in atmospheric chemistry.

Knowing what you know about the history of this facility and the current state of science, just how visionary was Bill Wiley?

He was right on track, and I believe his vision has been met. The future is very bright. With our solid capabilities in mass spectrometry, high-throughput proteomics, systems biology, computing and other areas, I believe we have an opportunity to bring a new DOE proteome research facility to PNNL within the next several years.

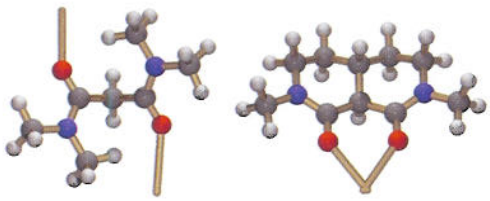
EMSL is established, the dream is reality, and with this potential new facility, we are truly bringing the Wiley vision full circle to create a new type of 21st century research capability. In looking back over EMSL's history, there is much credit to be given, much credit due. Many people have worked hard to make this facility an overwhelming success, and I think it's just going to get better. ●

EMSL generates impact beyond fundamental science

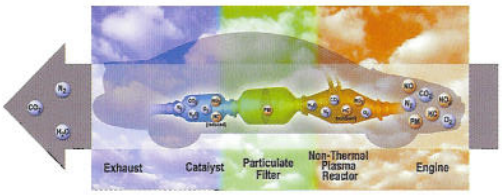
The research conducted at the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) does more than contribute to a basic understanding of the world around us. It also helps to improve the environment, ensure national security, advance health care, and promote clean energy through real-world applications. The following research projects demonstrate the diversity of EMSL's scientific contributions.

HostDesigner and designer materials—Advanced computational methods developed by researchers in EMSL are being used to identify new molecular structures that can be applied to speed environmental cleanup and also provide benefits in areas including pharmaceuticals and industrial processes. Using these methods, scientists have designed a new "ligand" or receptor that targets the f-block metal ions, a group of metal ions present in radioactive waste. Experimental studies have shown that the "designer" diamide ligand is 10 million times more efficient at removing f-block metals from process waste than conventional diamide ligands.

The ligand design methodology has been automated in a new computer software program called HostDesigner. This program was created specifically for the discovery of molecules that bind with metal ions—an application that is crucial for environmental cleanup and other industrial processes in which the objectives are to detect and recover metals. "Our ability to design molecules tailored for specific applications will save time and money by focusing research efforts on the most promising ligand structures," said Ben Hay, creator of HostDesigner.



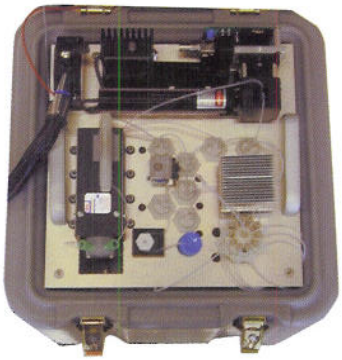
Computer-aided design of ligand architecture yields a dramatic enhancement of metal-ion affinity. The vectors on each oxygen atom, which indicate the direction required for optimal interaction with a metal ion, diverge in the conventional diamide structure (left) and converge in the computer-designed structure.



Engine Exhaust Aftertreatment System Based on Non-Thermal Plasma-Assisted Catalysis—Utilizing research at EMSL, scientists have developed an exhaust aftertreatment system based on non-thermal plasma-assisted catalysis for lean-burn diesel and gasoline engines. This system converts harmful oxides of nitrogen (NO_x) and particulate matter emitted from vehicle engines into components of clean air. In laboratory tests with a simulated gas mixture, this technology reduced the NO_x by nearly 100 percent. Tests with actual diesel engines have achieved greater than 75 percent NO_x reduction over a range of operating conditions and up to 50 percent particulate matter reduction. With the addition of an optional particulate filter, this system can reduce particulate emissions by up to 90 percent. The system performs well in the lean-burn conditions of energy-efficient diesel engines, where conventional three-way catalytic converters are inadequate. It also could easily be incorporated into existing vehicle tailpipe designs with few modifications and could be a retrofit option to decrease pollutants from older vehicles.

The system combines an electrically energized gas, or plasma, with specialized catalyst materials that selectively bring about important chemical reactions to reduce NO_x. "This concept of using a non-thermal plasma to activate catalysis has existed only for about 7 or 8 years," said Chuck Peden, who leads interfacial chemistry and engineering research. "Today it is recognized as a potential commercial solution." *See related story, page 16.*

BEADS (Biodetection Enabling Analyte Delivery System)—An automated system based on research conducted at EMSL purifies samples of soil, air and water. Called BEADS, for Biodetection Enabling Analyte Delivery System, it is being created for use in a biological warfare detector. BEADS cleans samples so that micro-organisms can be identified in places like food processing lines and water treatment plants. The system's sample preparation process can be used with existing detectors, which require a person to manually purify samples for identification. BEADS takes the person out of the process by using proprietary microfluidic systems and automated sample cleanup methods. It can be used in chemical, protein, nucleic acid or whole-cell detectors. ●



PNNL findings may help preserve Dungeness crab

A recent Pacific Northwest National Laboratory study has found that salinity levels in the Columbia River estuary may affect crab abundance in the river, a finding that may help protect Dungeness crab in the Columbia.

The study, sponsored by the Portland, Ore., District of the U.S. Army Corps of Engineers, sought to address the impact of regular maintenance dredging and a river deepening project on Dungeness crab. The Columbia River, which serves as a waterway for commerce from the West and Midwest, must be dredged yearly to keep the river deep enough for safe navigation. Dredging vessels ply the river from the ocean inland each summer, sucking up huge amounts of sediment – and the marine life living in it.

The Corps also plans to deepen the channel from 40 to 43 feet in the stretch from Portland to about three miles from the ocean, which will involve dredging. The Corps is increasing the authorized depth of the river so larger ships can call at ports on the Columbia. Currently, large ships carrying grain and other cargo cannot be fully loaded because there is not enough water for them to return to the ocean safely.

In looking at crab entrainment, or how many crab are trapped by dredges, PNNL researchers compared entrainment data and levels of salinity in the river, finding that lower levels of salinity meant less crabs. As salinity increased, so did crab abundance. "By timing dredging to coincide with lower levels of salinity, the Corps may be able to reduce the impact of dredging to crabs," said Walt Pearson of PNNL's Marine Sciences Laboratory. Several factors determine salinity, including location in the estuary, tides and river flow. These variables influence salinity daily, monthly, seasonally and yearly.

As a result of these findings, the Corps no longer considers dredging a threat to crab in some areas in the upper part of the Columbia River estuary because salinity levels are so low. Areas in the middle of the estuary vary in crab abundance because salinity levels vary.

PNNL researchers will refine their salinity-entrainment model before using it to further investigate salinity in the Columbia River and what it may mean for crab.

In addition, researchers used entrainment data from a summer 2002 study and a modified dredge impact model to make predictions about the number of crab that would be lost to entrainment during the deepening project. Applying a harvest rate, they estimated that the total crab that would be lost to crab fisheries would be equivalent to about one percent of one year's landings. ●

Chamber reveals chemical secrets

What if there were a magical chamber that could divulge the secrets of anything that was placed inside of it? Pacific Northwest National Laboratory has developed such a chamber—and while it won't divulge all secrets, it discloses key information about chemicals and compounds.

That information may be useful in addressing a wide range of issues that affect the environment and quality of life—everything from sick building syndrome and industrial emissions monitoring and control to sensor testing for homeland security applications.

PNNL's chamber, known as the Atmospheric Research Chamber, was developed in 2002. The chamber concept can be traced to PNNL's work in fate and transport studies, which revealed that there is still much to learn about how chemicals react in the environment.

The chamber actually is a large, room-sized set of dual chambers that analyzes chemical mixtures by subjecting the material to an assortment of tests. These tests, for example, characterize unknown chemical substances; expose chemicals to photo-oxidation or high humidity to mimic what might actually happen in the environment; and effectively monitor aerosols and molds. In addition, the chamber can be used to calibrate sensitive sensors or detectors for interferences like dusts, oils or other chemicals.

Teflon-lined and containing ultraviolet lights, reflective surfaces, sampling and purge ports, stirring fans and state-of-the-art analysis equipment, the chamber also provides information that could be used for determining chemical and/or biological sensor detection issues and validating computational modeling by performing actual experiments that can be done without expensive field tests. The chamber is able to measure high-boiling point, semivolatile chemicals without critical surface and line losses, shed new light on air pollution and health issues for civilian and military populations and provide improved understanding of hazardous waste discharges for more effective cleanup solutions.

"With the chamber's unique ability to work with semi-volatile chemicals and its powerful analytical capabilities, we feel that it can serve the needs of many different clients who would not be able to find the same capabilities elsewhere," said Kathy Probasco, senior research scientist. Probasco added the chamber's capabilities are now available to external clients and projects. ●

NOTABLE Achievements

PNNL honored for technology transfer

The Federal Laboratory Consortium has bestowed Awards for Excellence in Technology Transfer to Pacific Northwest National Laboratory's Acoustic Inspection Device, engine exhaust aftertreatment system and EMAdvantage© Emergency Management Software.

With a total of 54 awards, PNNL has been honored by the FLC more than any other federal laboratory since the recognition program began in 1984.

The Acoustic Inspection Device offers a noninvasive approach that allows rapid and reliable assessment of the contents of sealed, liquid-filled containers. The instrument can determine the characteristics of the liquid as well as detect foreign objects, contraband or explosives hidden inside the containers. In January 2002, PNNL signed a licensing agreement with Mehl, Griffin and Bartek, of Arlington, Va., to manufacture and sell the device to the U.S. Customs Service. A similar

version of the device is being used along borders in Eastern Europe to detect smuggled goods.

The engine exhaust aftertreatment system, developed by PNNL and industry partners, combines an electrically charged gas with a specialized catalyst to substantially reduce harmful vehicle exhaust emissions from diesel and gasoline engines. These reductions are critical to meeting government-mandated vehicle emissions and fuel economy requirements that will take effect toward the end of the decade. PNNL successfully transferred the technology to three organizations — Delphi Corp., Caterpillar Inc. and the Low Emissions Partnership of USCAR, a government-industry program that involves Ford Motor Co., DaimlerChrysler and General Motors Corp.

EMAdvantage© enables decision makers within an emergency operations center to make informed decisions and share information in real time with the larger emergency management community, including incident command centers, shelters, schools, hospitals, joint information centers and others involved in emergency planning and response activities. Recently, EMAdvantage© was customized to address situations specific to the oil industry, translated into Spanish and installed at the Minatitlan Refinery in Mexico where it is helping officials plan for and respond to a range of emergency events. ●

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