# Process Science and Engineering at Pacific Northwest National Laboratory



*Making Science Real*

*For close to four decades, Pacific Northwest National Laboratory's **Process Science and Engineering Division** has provided critical science and technology for practical applications. Using the resources afforded by a multidisciplinary national laboratory, and working closely with our clients, we deliver integrated technical solutions and products designed to manage all aspects of each client's problem.*

*Award-winning technologies, pioneered by PS&E scientists and engineers in areas such as waste treatment, pollution prevention and abatement, beneficial uses of nuclear materials, microtechnology, and bio-based products, are being used to address many of today's problems and challenges.*

*Our more than 225 process scientists, engineers, and specialists, using leading-edge equipment and facilities, form the foundation for building diverse technical teams to deliver specific solutions. These resources are enhanced by strategic alliances and collaboration with our clients and partners from industry, universities, national laboratories, and government agencies.*

# Technical Groups

**Advanced Processing and Applications**—We develop and demonstrate chemical and material processes and systems through such diverse environmental solutions as legacy nuclear material treatment and disposal and advanced materials for sensors and sustainable procesess.

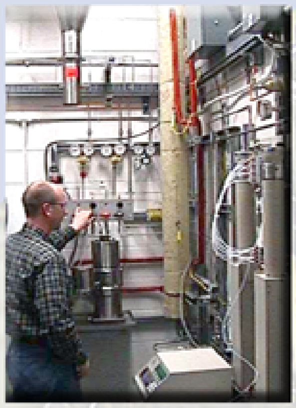
**Chemical and Biological Processes Development**—We provide solutions and products to meet our clients' needs through the development and application of process technologies tailored to resolving energy, security, and environmental issues.

**Fluid and Computational Engineering**—We address our clients problems involving multi-phase fluid dynamics, heat transport, mass transfer, and reactive transport over a wide range of length scales. We deliver solutions based on integrated expert analysis, experimentation, and computation.

**Radiochemical Science and Engineering**—We develop, test, and implement innovative processes for nuclear nonproliferation, environmental clean-up, advanced nuclear energy, homeland security, and the beneficial use of nuclear materials in medicine and industry.

## Process Engineering and Development—Science to Application

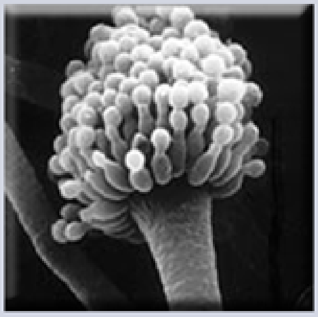
Promising scientific discoveries are evaluated and demonstrated on the laboratory, bench, and pilot scales, with a focus on developing energy and material balances and process flowsheets; evaluating preliminary process economics; and deploying innovative equipment and systems.



Process testing for system scale-up and demonstration.

## Bio-based Products

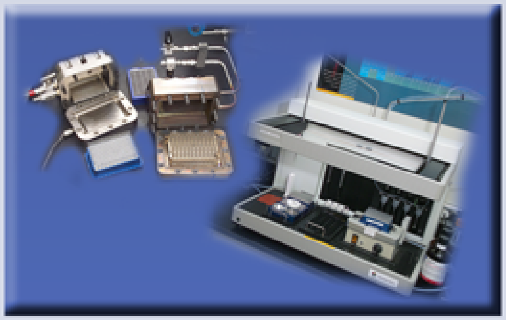
PS&E researchers are developing new processes and systems, as alternatives to petroleum-based methods, for manufacturing chemicals from readily available byproducts and wastes associated with agribusiness and food processing. Using technologies such as catalysis and fungal bioprocessing, low-value residues can be turned into valuable platform chemicals, like polyols, which serve as building blocks for such well-known commodities as antifreeze and polyester.



Based on fungal biotechnology, processes are being developed that use filamentous fungi to convert biomass to high-value chemical products.

## Catalysis and Reaction Engineering

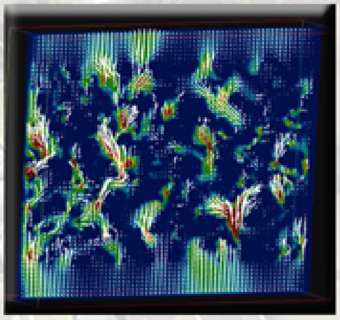
Innovative catalysis and reaction engineering solutions are being developed and applied to more efficiently use fossil energy; convert biomass and renewable feedstocks and chemicals; and reduce environmental emissions and waste streams. The evolution of these new technologies is enhanced through advanced catalyst characterization and testing facilities, such as high-throughput combinatorial catalysis systems, which provide more definitive information on the chemical reactions occurring on catalyst surfaces.



Combinational catalysis (CombiCat): up to 384 individual catalyst samples evaluated simultaneously.

## Fluid Dynamics

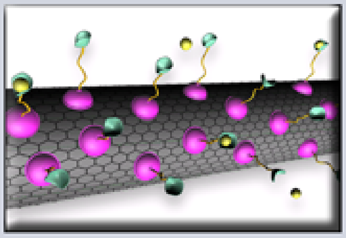
Large-scale numerical computation, micro- to pilot-scale experimentation, and engineering analyses are being applied to address processes involving multi-phase fluid dynamics, heat transport, mass transfer, and reactive transport over a wide range of length scales and liquid-solid systems. An important contribution to modeling fluid dynamics involved our application of the Lattice-Boltzmann (L-B) method to investigations of transport phenomena in flowing and thermal systems. Unlike conventional computational fluid dynamics methods, the L-B method efficiently computes the transport of momentum, heat, and mass at a huge number of closely spaced points and without having to specify the location of interfaces between liquid and vapor phases. With this ability, a more practical simulation is possible for many realistic situations.



Characterization and modeling of diesel particulate filter with Lattice-Boltzmann method.

## Functional Multi-scale Materials

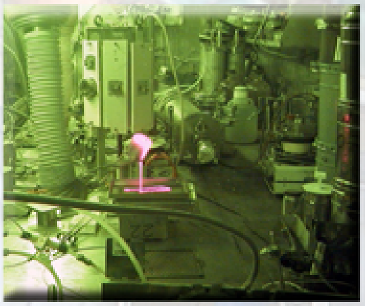
Functional multi-scale materials have highly specific surface chemistries coupled with several length scales to better facilitate coupled heat and mass transport. Applications include catalysis, separations, hydrogen generation and storage, and novel sensing platforms for chemical and nuclear threats. We design chemical ligands with high specificity for binding target molecules (such as environmental contaminants or chemical weapons agents), self-assemble them as functional groups on mesoporous media, consolidate those media first into microscale powders and then into macroscale engineered forms, and integrate them with hand-held portable detectors for real-time analysis.



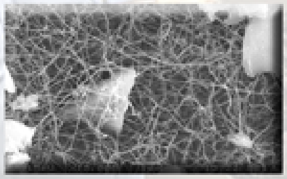
A new technique uses a super-critical fluid to load specially designed "anchor molecules" onto carbon nanotubes without compromising the strength or sensitivity of the tubes. With filaments ten-thousand times smaller than a human hair, carbon nanotubes exhibit unusual strength and unique electrical properties, and are efficient conductors of heat.

## Glass and Materials Science

Work by PS&E researchers was pivotal in advancing vitrification technology to the process designed for the Hanford Waste Treatment Plant (WTP). From the early glass characterization and waste form development work in the 1980s, these researchers, along with other PNNL colleagues, designed and integrated a wide range of vitrification systems, including the technologies that are the basis for the WTP facilities. Now, innovative materials and fabrication processes are being developed for applications such as glass-ceramic seals, optical/photonic media, sol-gels, polycerams (polymerceramic hybrid) improved sensor materials, and thin films.



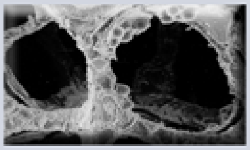
Waste vitrification testing in hot cell.



Chalcogenide nanowires, 25 to 900 nanometers in diameter, are being developed as tools for more sensitive photonic sensors and other infrared optics, as well as for use in antireflective coatings.

## Microtechnology Products

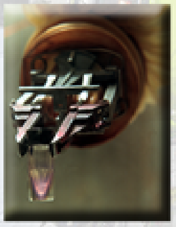
PS&E scientists and engineers helped create the field of microtechnology, which greatly increased heat and mass transfer rates, resulting in a new class of devices for chemical and thermal systems. Because they produce very high rates of heat and mass transfer, microchannels 10-100 microns thick, are key to the process-intensive, extremely efficient, microproducts being developed for energy, space exploration, national defense, chemical production, electronic devices, and instrumentation. Another groundbreaking achievement centered on developing catalysts with fast kinetics, then engineering them onto a support, followed by designing a microreactor around the catalyst to maximize catalyst performance. From there, steam reforming reactions were demonstrated in *milli-second* contact times, instead of seconds—a crucial enabling capability for generating hydrogen and syngas using microchannel technology.



Highly structured (on micron length scale) scaffolds/framework for supporting catalysts.

## Radiochemical Processing Research

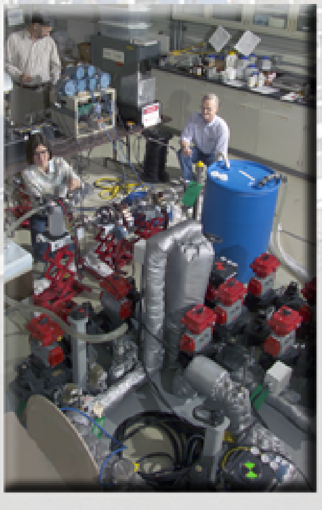
Through high-quality fundamental actinide science and strong academic collaborations, we are fostering a renewed focus on radiochemistry and irradiated materials research for providing solutions in nuclear nonproliferation, environmental cleanup and protection, advanced nuclear energy, and for use in medicine and industry. The technical capabilities that provide the background for this focus include radiochemical process engineering, irradiated materials characterization, and radiochemical separations and conversions—supported by a full-service, in-house analytical laboratory that provides a comprehensive suite of analytical instrumentation, with natural linkages in process modeling, colloidal particle interfacial dispersion, and surface science—all while maintaining stewardship for one of the few remaining multipurpose Category 2 nuclear R&D hot cell facilities in the U.S. Department of Energy complex.



Using separation and purification processes, researchers produce a reliable supply of ultrapure yttrium-90, a beta-emitting radioisotope widely used for cancer therapy in conjunction with monoclonal antibodies. Separation and purification processes are also making bismuth-213, an alpha-emitting radioisotope, more readily available for advancements in cancer treatments.

## Waste Treatment

Our researchers have an extensive role in support of Hanford Site operations and cleanup. This work has spanned waste separation, processing, and immobilization technologies, as well as development, scale-up, and deployment of first-of-a-kind processes and computational modeling tools to address environmental, tank safety, and system design and operational safety issues. PS&E researchers provided the scientific basis, such as chemical and physical properties, behavior, and interaction of materials, and direction to projects, in support of the Hanford Tank Safety Program, which closed the hydrogen gas generation, ferrocyanide, and organic-nitrate unresolved safety questions. Closing these safety questions allowed tank waste cleanup operations to continue. At the Hanford K Basins, testing and engineering evaluations by PS&E researchers helped establish defensible design and safety basis parameters for processing and dry storage of spent nuclear fuel and sludge.



A process monitor system that collects and processes information on chemical and physical characteristics of complex waste streams was developed in support of salt cake retrieval activities for Hanford tank wastes. This unique system, which can also be applied to a variety of industrial waste streams, is the first example of a real-time monitoring of tank waste composition and cumulative status during processing.

# Awards

PS&E research teams have earned numerous honors, including a combined 30 awards from *Research and Development* Magazine (R&D 100), the Federal Laboratory Consortium (technology transfer), and the Presidential Green Chemistry Challenge.

# Key Facilities

**The Process Science and Engineering Division is a laboratory-intensive organization, with staff helping to establish capabilities and generate technology advancements in key research and development facilities.**

### Applied Process Engineering Laboratory

The Applied Process Engineering Laboratory (APEL) is an advanced user facility with state-of-the-art engineering and manufacturing scale testing and demonstration capabilities, as well as wet, bio, and electronics laboratories. Prototypes or pilot plants can be tested and initial manufacturing conducted using APEL's utilities, services, and permits.

### Bioproducts, Science and Engineering Laboratory

Scheduled to be completed in 2007, the Bioproducts Sciences and Engineering Laboratory (BSEL) will provide a state-of-the-art facility for research to convert low-value agricultural byproducts and residues such as culls, hulls, peelings, straw, and manure into value-added chemicals for products like plastics solvents, fibers, pharmaceuticals, nutriceuticals, and fuel additives. The facility will also include classrooms and laboratories for science and education and an expanding viticulture and enology program at Washington State University Tri-Cities.

### Environmental Molecular Sciences Laboratory

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a DOE National Scientific User Facility and research organization that houses some of the world's most cutting-edge research equipment. Since its inception in 1997, the 200,000-square-foot facility has hosted more than 5500 visiting scientists, professors, and others, who come from academia, research and development laboratories, and industry. A resident staff of 200 includes experts in the areas of chemical, physical, biological, and computational sciences.

### Oregon Nanoscience and Microtechnologies Institute/Microproducts Breakthrough Institute

The Oregon Nanoscience and Microtechnologies Institute (ONAMI) is Oregon's first "Signature Research Center" for the purpose of growing research and commercialization to accelerate innovation-based economic development in Oregon and the Pacific Northwest. It is also an unprecedented and powerful collaboration involving Oregon's three public research universities - Oregon State University, Portland State University, University of Oregon; the Pacific Northwest National Laboratory (Richland, WA); the state of Oregon; selected researchers from the Oregon Graduate Institute and the Oregon Health and Sciences University; and the world-leading "Silicon Forest" high technology industry cluster of Oregon and southwest Washington.

The Microproducts Breakthrough Institute (MBI) is a joint venture between OSU's Microtechnology-based Energy and Chemical Systems (MECS) and PNNL's Micro Chemical and Thermal Systems (MicroCATS) program. The MBI's focus includes helping to develop and commercialize ONAMI-related technologies. The facility features unique equipment and processes for micropatterning, micro laminate bonding, micromolding, and microreactor fabrication. PS&E plans to have 10-20 staff located at the MBI facility in Corvallis, Oregon by FY 09.

### Radiochemical Processing Laboratory

The Radiochemical Processing Laboratory is a DOE Hazard Category 2 facility for work with microgram to kilogram quantities of fissionable and nonfissionable radioactive materials ranging from picocurie to megacurie levels of activity. The facility contains extensive wet laboratories, shielded glove boxes, wet radiochemistry fume hoods, and associated equipment for conducting radiochemical separations, radioanalytical measurements, radioactive materials characterization, and radioactive and hazardous waste management.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