TECHNOLOGY

Catalytically Converted

Chemistry, fundamental and applied, reaches a critical mass at PNNL

by Bill Cannon

Life began as a series of chemical reactions and is sustained by them. In the industrial age, the quality of that life, for human beings at least, has depended largely on our ability to direct and control chemical reactions that are used to create the products and processes that people have come to expect, from life-saving pharmaceuticals to new transportation technologies. Playing a central role in the control of those reactions are chemical substances called catalysts.

"Chemists haven't done themselves many favors," says Douglas Ray, chemistry division head at the Pacific Northwest National Laboratory in Richland, Wash.

"They've left the discussion of materials to the materials scientists. But all catalysts"—traditionally defined as substances that modify chemical reaction rates and that remain unchanged afterward—"are materials, right?"

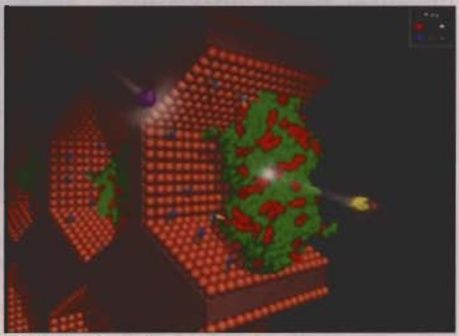
Ray emphasizes "it's not just about materials; it's also about the chemistry, the functionality of materials, the transformation of reactants into products."

Last year Ray went to the Hill to testify to Washington's congressional delegation about what the nation stands to gain by stepping up its research investment in catalysis.

Catalysis, he told the lawmakers, is "a means of changing the rates of chemical reactions, increasing the amounts of desirable products and reducing the yield of undesirable products." The effort, he said, should be directed at inventing new catalysts to efficiently produce materials and alternative fuels, including hydrogen; to increase efficiency of transportation and manufacturing; to mitigate climate change; to protect citizens from release of toxic substances and infectious agents; and to create new pharmaceuticals.

Catalysis at PNNL

Now Ray is testifying in the less rarefied air outside his office, in a hallway of the lab's Environmental Technology Building. He motions to a printed mural, drawing attention to



PNNL's technology called self-assembled monolayer on mesoporous silica, or SAMMS, enables an enzyme called OPH to become twice as active and extremely stable. The immobilized enzyme is promising for detecting, immobilizing, and neutralizing harmful agents.

the section called "Control of Chemical Transformations."

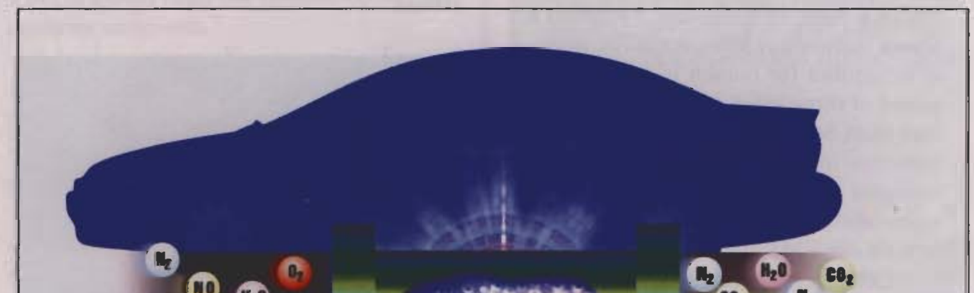
The mural depicts a few of PNNL's successes in the world of catalysis. One of its biggest stars, and noted by the journal *Science*, is SAMMS, for "self-assembled monolayer on mesoporous silica." These crafty catalysts rely on an enzyme embedded in nanoscale materials, rendering that enzyme, called organophosphorus hydrolase, twice as active and stable. The immobilized enzyme holds great promise for detecting, immobilizing and neutralizing harmful chemicals.

In another area, PNNL nanotechnologists have synthesized photocatalysts that convert visible light into chemical energy—for example, splitting water to generate molecular hydrogen.

In the environmental arena, PNNL research has been directed toward catalysts to help convert harmful nitrogen oxides (NOx) to benign nitrogen.

If most people have heard of catalysis at all, it's from the phrase "catalytic converter," a device that scrubs auto exhaust of many of its more odious and environmentally unhealthy properties. PNNL scientists have spent more than a decade studying the fundamental science of catalytic converters, work that has drawn the attention and support of the Big Three automakers, among others.

Recently, PNNL has also developed a novel twist on vehicle exhaust-cleansing, with a new system that converts diesel engine exhaust loaded with NOx—the major ingredient in smog and a contributor to the acid rain and ozone problems—to harmless gas. Diesel exhaust flows into a device filled with charged gases, a non-thermal plasma reactor, and is then acted upon by a catalyst that reduces the NOx into harmless nitrogen, which is what the air we breathe is mostly made of.



PNNL and industry collaborators have developed a system that converts vehicle exhaust loaded with nitric oxides to harmless gas. Exhaust flows into a non-thermal plasma reactor and is converted to nitrogen dioxide, which is then acted upon by a catalyst that reduces it into harmless nitrogen.

Powerful tools

Across the street from Ray's building, at the lab's W. R. Wiley Environmental Molecular Sciences Laboratory, or EMSL, Chuck Peden fiddles with a PowerPoint compilation of catalysis work at the lab.

The abundance of slides at Peden's command attests to the amount and diversity of projects that come in at a pace of $8 million a year for catalysis-related research, and that figure doesn't include proprietary work for industrial clients. The work ranges from fundamental catalysis science and process development using microchannel reactors to catalytic materials for solid-oxide fuel cells and solid-acid catalysts of interest in petroleum refining.

All of this is made possible by the federal agency for which Battelle Memorial Institute manages the lab, the Department of Energy. The DOE has invested heavily in tools of discovery at EMSL. Among the more prominent is one of the world's fastest unclassified-science supercomputers, ideally suited for running impossibly complex chemical-transformation simulations, which proved instrumental in a three-year, $6.6-million, multi-institution DOE grant that PNNL won last fall to model and build new metal oxide catalysts on an atomic scale.

Add to that list a suite of spectroscopic labs, specialized laser and visualization machinery, and the world's most powerful magnetic-resonance instruments for probing the details of chemical reactions in real time and unprecedented detail, plus more than four dozen resident investigators and hundreds of visiting scientists from around the world, and you begin to get a sense of the activity surrounding what the lab lumps under the rubric "heterogeneous catalysis."

As one reviewer recently put it, "PNNL has the people and the facilities to become the best center for catalyst studies in the world. In other words, I suggest DOE consider PNNL as a potential national resource in this area."

If PNNL has a catalysis guru, it is Peden. For one thing, he has worked exhaustively, as it were, on the exhaust research, and now he and colleagues Chris Aardahl and Yong Wang are attempting to put the plasma reactor concept to larger, industrial purposes. In the past year they've devised a portable reactor system that can be moved from lab to lab where specific analytic tools reside. They also built a reactor that can be operated at higher-than-atmospheric air pressures suitable for the synthetic chemistry that interests them. Typically, plasma chemistry is performed at atmospheric or less-than-atmospheric pressure. They believe their experimental setup to be a first.

The idea is to increase the efficiency of chemical reactions employed in the chemical industry, so that smaller quantities of bulk chemicals are needed to achieve the desired compounds. The work could have large ramifications for the industry–and for those who live near industrial plants.

"If you can get the same amount of product from much less material introduced into the process," Peden says, "it obviates the need for a single huge factory, a concentration of waste products, and a lot of shipping. You can have smaller, low-waste chemical boutiques," he says, "where the products are needed."

From theory to practice and economic impact

Not far from EMSL as the magpie flies, the fruit of basic research is put to the test at the Exhaust Emission Science Laboratory. The lab applies catalysis breakthroughs like those made at EMSL to emission-treatment technology. Emission lab director George Muntean has noted that many of the applications are built around the principle of improving the selectivity of a given "reductant," a substance that chemically reacts with harmful nitrogen oxide molecules to convert it back to components of clean-air nitrogen, oxygen and water.

In this context, surfaces where nitrogen oxides react with the reductant play a crucial role. Muntean likes to point out that in such a reaction "there are no moving parts." Dirty gas flows over a large surface and comes out clean on the other end. The key to advancing the application is learning, at the most fundamental level possible, how molecules arrange themselves on the surface, how they react with the surface, and how the surface changes.

To ensure the relevance of the work, the emissions lab takes on industry partners. For example, under a cooperative research and development agreement with Caterpillar, researchers have devised a "sulfur trap" to remove catalysis-interfering sulfur from the exhaust of heavy-duty diesel engines.

Peden points out that the worldwide economic impact of catalysis is on the order of $10 trillion a year. Ray would like to see a larger share of that concentrated in this corner of the country, and "someday" isn't in his vocabulary.

"In no other area can the nanotechnology revolution have such an immediate payoff," Ray told Washington's congressional delegation. "Increased federal investment in catalysis R&D benefits the Northwest in multiple ways: the region's research institutions will receive enhanced federal funding, the region's workforce will become better trained in this important area, and new discoveries will result in new jobs." ■

The Exhaust Emission Science Laboratory integrates emissions research at PNNL.

Bill Cannon recently returned to the region as a science communications specialist for PNNL.