Pacific Northwest NATIONAL LABORATORY

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The Institute for Interfacial Catalysis is supporting PNNL's Energy Conversion Initiative in studying coal gasification and direct liquefaction to provide power and transportation fuels with minimum emissions.

Pacific Northwest National Laboratory:

INSTITUTE FOR INTERFACIAL CATALYSIS

Coal-to-Liquid-Fuels Research

Many high-volume, high-quality sources of crude oil are geographically located in regions that are relatively insecure politically and where prices are not influenced by U.S. markets. While high-purity, high-pressure hydrogen may be the fuel/energy carrier in the long term, strategies to help supply and maintain the nation's liquid hydrocarbon infrastructure with compatible transportation fuels are critical in the near term.

Focusing on indigenous coal and recognizing the constraints of air and water neutrality, Pacific Northwest National Laboratory's (PNNL's) Institute for Interfacial Catalysis is addressing the direct and indirect conversion of coal to liquid transportation fuels.

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

INDIRECT LIQUEFACTION: MORE VALUABLE PRODUCTS FOR LESS COST

Producing diesel and other fuels from coal can be done through converting coal to syngas, a combination of carbon monoxide, hydrogen, carbon dioxide, and methane. The syngas is reacted through the Fischer-Tropsch synthesis (FTS) to produce hydrocarbons that can be refined into transportation fuels. By increasing the quantity of high-quality fuels from coal while reducing the costs, research into this process could help ease the country's dependence on foreign oil.

Our researchers are exploring novel concepts to control product distribution in FTS. By applying our strengths in FTS catalysts, nanoscale catalyst synthesis, reactor design, and monolith catalyst integration, we are exploring ways to reduce diffusion length and minimize re-adsorption of olefins to narrow the product distribution, achieving more gasoline and diesel.

U.S. DEPARTMENT OF ENERGY

DIRECT LIQUEFACTION: REFINERY-ACCEPTABLE PRODUCTS

By improving the catalysts used in directly converting coal into liquid hydrocarbons, without the generation of the intermediate syngas, less power could be required to produce a product suitable for upgrading in existing petroleum refineries.

Researchers are developing sophisticated methods to characterize the structure of certain coal types, and to identify specific sites within the coal structure that are most susceptible to reaction with catalysts. Such an approach could reduce energy requirements and improve yields of desired products.

Separately, researchers are studying inexpensive nanoparticulate iron-based catalysts and

- Testing catalyst activity and selectivity using model compounds and well-characterized coals
- Evaluating hydrothermal processes for both catalyst nucleation and liquids extraction
- Testing supercritical carbon dioxide as a solvent for extracting low molecular weight coal components, and as a medium for catalyst delivery and coal pulverization.

REDUCED POLLUTANTS FROM COAL USE

While coal is an abundant natural resource, its combustion or gasification produces both toxic pollutants and greenhouse gases. By developing adsorbents to capture the pollutants (mercury, sulfur, arsenic, and other harmful gases), our researchers are striving not only to reduce the quantity of emitted gases but also to maximize the thermal efficiency of the cleanup.

We are developing materials to remove the greenhouse gas carbon dioxide from process streams. For example, a special class of calixarenes, developed by researchers at PNNL and the University of Missouri-Columbia, appears to be very promising for separating carbon dioxide from gas mixtures. A subsequent step that also involves PNNL researchers is the safe sequestration of carbon dioxide once captured.

ABOUT PNNL

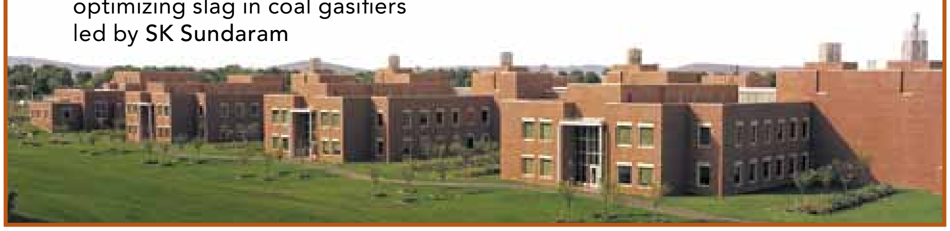
Pacific Northwest National Laboratory, a U.S. Department of Energy Office of Science laboratory, solves complex problems in energy, the environment, and national security by advancing the understanding of science. PNNL employs more than 4000 staff, has a business volume of $750 million, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

▶ EXPLORING OPPORTUNITIES IN COAL RESEARCH

The Institute for **Interfacial Catalysis** supports innovative coal research projects under PNNL's Energy Conversion Initiative, including

- Tailoring of Fischer-Tropsch synthesis product distribution using monolith catalysts led by **Yong Wang**
- Catalytic chemistry of the weak bonds in lignins and lignites led by **Conrad Zhang**
- Improved catalysts for direct coal liquefaction led by **John Linehan**
- Low-cost, small-scale hydrogen production and purification from natural gas led by **Yong Wang**
- Advanced gasifier modeling led by **Vladimir Korolev**
- Fuel chemistry relationships to fuel system wear led by **Thomas Gallant**
- Measuring, modeling, and optimizing slag in coal gasifiers led by **SK Sundaram**
- Real-time in-situ millimeter wave sensors for gasifiers led by **SK Sundaram**
- Liquid fuel synthesis and reactor modeling led by **David Rector**
- Deep desulfurization of hot coal gas led by **Liyu Li**
- Novel carbon dioxide capture processes using organic clathrates led by **Pete McGrail**
- Design, synthesis, and testing of novel high-temperature sorbents for removing mercury species led by **Glen Fryxell**.

To produce liquid fuels from coal, we draw on our expertise in chemical and materials sciences, catalysis and reaction engineering, process development and engineering analyses, technology assessments, sensors, and computational modeling.



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