

Advanced Analysis: Enabling a New Green Industry

Developing sustainable technologies for renewable fuels and chemicals is the goal of Pacific Northwest National Laboratory's advanced analysis team. We examine the effects of practices used to create renewables from the global scale all the way to the molecular scale.

Global. We create models that assess the pressure placed on global systems—land, water and climate—from large-scale implementation of new technologies.

Farm. Researchers couple high-resolution, geologic information system models with physical models that examine suitable land, nutrients, climate, water and infrastructure to evaluate biomass resource production and use.

Conversion. Engineers perform technoeconomic and life cycle analyses that help us understand conversion costs and where research and development can have the greatest impact on reducing costs while optimizing sustainability.

Molecular. Researchers take advantage of molecular simulations, which use theory and energetic calculations. From this, we are able to:

- » Obtain information needed for process engineering
- » Understand reaction mechanisms and catalysis sites to design better catalysts
- » Understand metabolic pathways that allow us to improve biological processes.

EXPERTISE AND CAPABILITIES

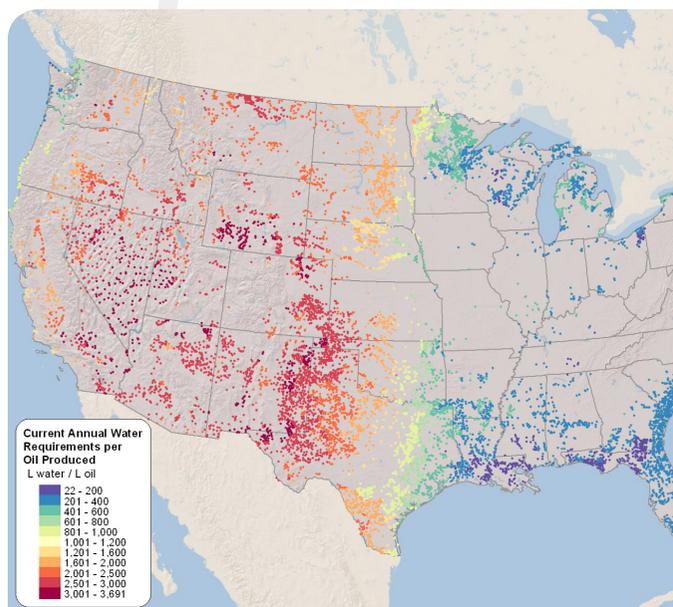
The Global Change Assessment Model. The Global Change Assessment Model, GCAM, offers cutting-edge analysis capabilities. GCAM:

- » Defines the scale of bioenergy systems in a long-term international context
- » Simulates economic competition of bioenergy technologies across all energy sectors
- » Examines production of bioenergy in the context of international agriculture and land use
- » Considers the impact of bioenergy on land and emissions, crop prices, and is moving to include water.

Biomass Assessment Tool. PNNL has developed a unique high-resolution spatio-temporal Biomass Assessment Tool (BAT) that asks critical questions related to the amount of energy that can be produced, where production can occur, and how much land, water and nutrient resources will be required. This research is being used to support DOE and industry. Its assessment of algae has been recognized by the American Geophysical Union, used in a recent National Research Council Report, and cited by President Obama in a 2012 energy policy speech.

Technoeconomic and Life Cycle Analysis. PNNL's technology analysts use the leading process simulators to evaluate emerging technologies in the context of a bio-refinery. Understanding the technical, environmental, and

impacts



PROCESS AND LIFE CYCLE MODELS

PNNL's suite of advanced analysis tools are being used to:

- » Perform assessments to understand how much biomass can be grown in the western U.S. and the impact of climate change on biomass growth
- » Determine how much algae can be produced and the best locations for production, such as the Gulf Coast
- » Engineer improved fungal systems to connect biomass to novel fuel and chemical precursors, such as polyketides, terpenes and organic acids
- » Improve our understanding of catalytic sites and develop new materials to transform biomass to fuels and chemicals.



economic performance of the current state of an emerging technology, then comparing it to theoretical and practical engineering limitations, allows analysts to identify research and development that could reduce costs and environmental impacts. Common simulation platforms used by PNNL analysts include Aspen Plus®, CHEMCAD, and SimaPro.

Molecular Simulation. PNNL's biomass group cultivates a robust dialogue with experts at EMSL, the Environmental Molecular Sciences Laboratory, a DOE user facility on the PNNL campus. EMSL expertise includes Molecular Science Software Suite, a comprehensive, integrated set of tools that enables scientists to understand complex biomass conversion at the molecular level.

DELIVERING IMPACT

PNNL's suite of in-house analysis tools includes:

- » Liquefaction: fast pyrolysis, catalytic fast pyrolysis and hydrothermal liquefaction
- » Gasification and catalytic hydrothermal gasification: mixed alcohols, Fisher-Tropsch liquids, or dimethyl ether (DME), methanol to gasoline (MTG), and methanol to olefins (MTO)
- » Fermentation: ethanol, hydrocarbons, organic acid
- » Emerging technologies being developed with industry.

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ABOUT BSEL

The Bioproducts, Sciences, and Engineering Laboratory (BSEL) is a multipurpose R&D facility that includes:

- » Modern laboratories for fungal strain and bioprocess development and optimization
- » 2,500-square-foot high-bay biorefinery for technology scale up
- » Analytical chemistry lab equipped with a wide array of analytical instruments.

COLLABORATIONS

PNNL collaborates with multiple industrial partners to keep its research relevant to the needs of industry and to facilitate technology transfer to the public domain. We also have major leadership roles in the Joint BioEnergy Institute (JBEI), DOE's National Advanced Biofuels Consortium (NABC) and National Alliance for Advanced Biofuels (NAABB). We partner with world-class regional, national and international universities and have active collaborations with other national laboratories.

ABOUT JGCRI

The Joint Global Change Research Institute (JGCRI) houses an interdisciplinary team dedicated to understanding the problems of global climate change and their potential solutions. Joint Institute staff bring decades of experience and expertise to bear in science, technology, economics, and policy. JGCRI is a joint venture between PNNL and the University of Maryland. To learn more about JGCRI, visit <http://www.globalchange.umd.edu/>.

ABOUT EMSL

EMSL, the Environmental Molecular Sciences Laboratory, is a U.S. Department of Energy national scientific user facility located at PNNL. EMSL provides integrated experimental and computational resources for discovery and technological innovations. To learn more about EMSL, visit <http://www.emsl.pnnl.gov/>.

ABOUT PNNL

PNNL's biomass conversion work is an important element in a wider portfolio of research and development funded by the U.S. Department of Energy, other federal agencies and the private sector. PNNL is a DOE Office of Science National Laboratory where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems in energy, national security and the environment. To learn more about PNNL, visit <http://www.pnnl.gov/>.


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