Quarterly Update

National Bioenergy Center Biochemical Platform Integration Project

Biomass

Biomass Program—Sustainable Fuels, Chemicals, Materials, and Power

July-September 2006, #12

The Biochemical Processing Integration Task focuses on integrating the processing steps involved in enzyme-based lignocellulose conversion technology. This project supports the U.S. Department of Energy's efforts to foster development, demonstration, and deployment of "biochemical platform" biorefineries that produce inexpensive commodity sugars and fuel ethanol, as well as a variety of other fuel and chemical products, from abundant renewable lignocellulosic biomass.

The National Renewable Energy Laboratory manages this project for DOE's Office of the Biomass Program. Information on the Biomass Program is available at [Biomass Program]

To discuss information in this update or for further information on the Biochemical Processing Integration Task, contact Daniel Schell at NREL, phone (303) 384-6869, email dan_schell@nrel.gov

29th Symposium on Biotechnology for Fuels and Chemicals.

Mark your calendars as the 29th Symposium is rapidly approaching with abstracts due in early December. The Symposium will be held in downtown Denver, CO at the Adam's Mark Hotel from April 29 – May 2, 2007. Meeting and abstract submittal information can be found at the following web site: http://www.simhq.org/meetings/07_symposium.aspx.

This year's sessions are listed below:

Session 1A: Feedstock Genomics and Development
This session will highlight advances in plant breeding and development to improve plant architectural, compositional or physiological characteristics to enhance the quality and value of the renewable feedstocks base.

Session 1B: Microbial Catalysis and Engineering
Presentations will focus on progress in discovery and/or development of microorganisms for improved production of fuels and chemicals.

Session 2: Enzyme Catalysis and Engineering
This session will highlight advances in enzyme discovery, characterization and/or modification to improve performance, as well as on improvements in cost effectively producing and applying enzymes to fuels and chemicals production processes.

Session 3: Bioprocess and Separations R&D
Presentations will focus on improvements in the efficient integration of reactor and process design and engineering with microbiology, biochemistry and chemistry to develop more economical bioprocesses and unit operations to produce and/or recover fuels and chemicals

Session 4: Biorefineries and Advanced System Concepts
This session will highlight lessons learned and progress being made in today's biorefining operations as well as describe concepts for increasing the efficiency and economic viability of future biorefineries.

Session 5A: Feedstock Preprocessing and Supply Logistics
Presentations will focus on innovations in agronomic cultivation, harvesting, storage and transportation methods, including environmental and economic impacts.

Session 5B: Feedstock Fractionation & Hydrolysis
This session will highlight progress in the development and demonstration of novel reactor configurations and more economical processing approaches for pretreating and saccharifying biomass.

Session 6: Industrial Biofuels and Biobased Products
Presentations will focus on improvements in the development, demonstration and commercialization of biologically-based processes for the economical production of fuels, chemicals and other value-added bioproducts.

Special Session A: Policy Drivers and International Development of Biofuels
A panel of speakers will address the policy drivers necessary to further the international development of 2nd-generation biofuels. Participants may consider advances in 1st-generation fuels, technological challenges and solutions, and innovative policy tools to support lignocellulosic biofuels development.

Special Session B: Compositional and Structural Analysis of Biomass
Invited presentations will highlight advances in the accuracy, precision, comprehensiveness, and cost of characterizing the structure and composition of lignocellulosic feedstocks, processing intermediates and residues.

R&D Progress

Improving Measurement of Lignin in Pretreated Biomass. We recently measured lignin mass balance closures of greater than 150% during dilute acid pretreatment of corn stover. These results suggest that lignin compositional measurements of raw and/or pretreated corn stover were incorrect. Therefore, we applied a spectroscopic technique, solid-state nuclear magnetic resonance spectroscopy (NMR), as an alternative method of measuring lignin content of these materials. The spectroscopic lignin values for stover pretreated over a wide range of severities were compared to values obtained from a traditional wet chemical Klason analysis. The NMR lignin values ranged from 17.0% to 30.8% compared to a range of 23.5% to 37.7% using the Klason lignin method. Mass balance closure for lignin using NMR-determined lignin values ranged from 94.6% to 140.8%, with a mean mass closure of 124.4%, compared to a range of 142.5% to 181.0%, with a mean mass closure of 162.5% for the Klason method. We did not find any evidence that lignin measurements in raw stover were wrong, suggesting that the chemical structure of pretreated material is altered enough during pretreatment so that the traditional method is no longer accurate. Possible explanations include carbohydrates that are protected by the remaining lignin and are not hydrolyzed during the Klason procedure, or there are lignin-carbohydrate linkages that are resistant to acid hydrolysis and these carbohydrate components are not released during the Klason measurement. Solid state NMR spectra showed that much of the protein is solubilized during acid pretreatment suggesting that the error is associated with some other cell wall component condensing along with lignin during the Klason procedure. It will become increasingly important to have accurate measurements of lignin content in pretreated and enzymatically hydrolyzed residues as their lignin content will determine the energy that can be derived from combustion or thermochemical conversion of these materials.

Related Activities

Work in NREL's Pretreatment and Enzymatic Hydrolysis Task Investigates Other Pretreatment Chemistries and Feedstocks. Recent work looked at the effect of different pretreatment conditions spanning acidic, neutral and alkaline chemistries and temperatures of 150 °C to 190 °C on pretreatment and enzymatic hydrolysis of switchgrass and wheat straw. The results will be reported as a relative reactivity, which is a function of the yield of both glucose and xylose released by biomass pretreatment and enzymatic hydrolysis. This methodology allows rapid screening of different biomass feedstocks treated at a variety of conditions. The goal is to identify a range of conditions that effectively hydrolyze all biomass carbohydrates. These results will also provide baseline data for comparison with the relative reactivity of other feedstocks treated using the same methodology. The results of this study will be reported at a future date.

Two of NREL's Computational Studies in the *Journal of Physical Chemistry* Increase Fundamental Understanding of Sugar Hydrolysis. A paper describing the quantum mechanical modeling of the acid catalyzed dehydration of glycerol was recently published in the *Journal of Physical Chemistry*, and another paper describing quantum mechanical modeling of the acid catalyzed decomposition of xylose was accepted in the same journal. The glycerol paper, "Mechanisms of Glycerol Dehydration," (M. R. Nimlos, S. J. Blanksby, X. Qian, M. E. Himmel, and D. K. Johnson, *Journal of Physical Chemistry A,* 2006, *110*, 6145-6156) described an extensive model study of the triol functional group found in glycerol and in many sugars. This study determined the reaction energies and barriers for several different reaction mechanisms. Some of the same mechanisms were investigated in the second paper, "Energetics of Xylose Decomposition as Determined Using Quantum Mechanical Modeling," (M. R. Nimlos, X. Qian, M. Davis, M. E. Himmel, and D. K. Johnson, *Journal of Physical Chemistry A,* In Press), which compared reaction barriers for the decomposition of xylose. This second study determined which of two possible reaction pathways to the formation of furfural is most likely in acidic solutions. In addition, the reaction barrier was determined for the likely mechanism for formic acid formation. Both of these reactions could represent significant sugar loss mechanisms and understanding these reactions may lead to strategies to reduce and/or eliminate sugar losses that occur during acid-catalyzed pretreatment of biomass.

Biochemical Processing Integration Task Information. Web-based information on the process integration project, including presentations made at the most recent stage gate interim review meeting, can be found at the following link (Process Integration Project Information). A discussion of how Stage Gate management is used in the Biomass Program is also available at this site (Stage Gate Management).

Produced for the

U.S. Department of Energy
Energy Efficiency and Renewable Energy

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1000 Independence Avenue, SW, Washington, DC 20585
by the National Renewable Energy Laboratory, a DOE national laboratory

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Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

DOE/GO-102006-2093 • October 2006

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