Frontiers in Biorefining

Biobased Products from Renewable Carbon

ABSTRACTS

Thursday, October 21, 2010

Session 3B: Advances in Analytical Techniques

EFFECT OF PRETREATMENT ON BIOMASS STRUCTURE AND CELLULOSE PROPERTIES

David Johnson

Biosciences Center
National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401-3305

davisonbh@ornl.gov

The structure and chemical composition of plant biomass has evolved to make the cellulose recalcitrant to hydrolysis by cellulase enzymes. Contributing factors to the recalcitrance of lignocellulosic biomass include cell structure, liquid penetration into the plant cell wall, hemicellulose and cellulose chemical structures, and lignification. Enzymatic conversion of lignocellulosic biomass requires an effective pretreatment to enable efficient cellulase action. Dilute acid pretreatment substantially increases the accessibility of the cellulose to hydrolytic enzymes and decreases the recalcitrance of the cellulose to hydrolysis. Using a variety of tools, we have developed a better understanding of how the pretreatment process affects biomass structure and cellulose properties that impact on its digestibility. Characteristics such as cellulose accessibility, crystallinity, morphology and molecular weight are monitored to ascertain the effects of pretreatment in addition to other factors including substrate porosity and particle size. Microscopic imaging can indicate changes in lignin and xylan distribution in the plant cell wall that are also important.

CHARACTERIZATION OF BIOMASS FOR UNDERSTANDING RECALCITRANCE: APPROACHES FROM THE BIOENERGY SCIENCE CENTER

Brian H. Davison[1], *Paul Gilna*[1], *Suzy Fowler*[1], *and Mark Davis*[2]

BioEnergy Science Center and [1]Oak Ridge National Laboratory
Oak Ridge, TN

And

[2]National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401-3305

davisonbh@ornl.gov

The challenge of producing and converting sustainable cellulosic biomass into fuels has the opportunity for science and technology to make an appreciable national impact in the next 20 years. However, the recalcitrance of biomass to conversion (or the ability to access the sugars and other monomers in order to make fuels or other products) is one of the major challenges. This is a central theme of the BioEnergy Science Center (www.bioenergycenter.org). Transformative advances to understand biomass recalcitrance will require detailed knowledge of (1) the chemical and physical properties of biomass that influence recalcitrance, (2) how these properties can be altered by engineering plant biosynthetic pathways, and (3) how biomass properties change during pretreatment and how such changes affect biomass-biocatalyst interactions during deconstruction by enzymes and microorganisms. The BESC Characterization Team is developing and applying a suite of chemical, physical, and imaging methods to identify relationships between biomass structure, enzyme and microbial interactions, and recalcitrance to test and further refine our understanding of the key features hindering the economic utilization of biomass resources.

REAL-TIME VISUALIZATION OF LIGNOCELLULOSE DECONSTRUCTION BY INTEGRATION OF NEUTRON SCATTERING, SPECTROSCOPY, MICROSCOPY, AND COMPUTER SIMULATION

Barbara R. Evans[1], Sai Venkatesh Pingali[1], Jeremy C. Smith[1,3], Loukas Petridis[1], Volker Urban[1], Dean A. Myles[1], William T. Heller[1], Hugh M. O'Neill[1], Junhong He[1], Art Ragauskas[2], Marcus Foston[2], Ida Lee[1,3], Brian H. Davison[1]*

[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee
[2]Institute of Paper Science and Technology, Georgia Institute of Technology, Atlanta, Georgia
[3]University of Tennessee, Knoxville, Tennessee

*Oak Ridge National Laboratory
1 Bethel Valley Road
4500N MS 6194
Oak Ridge, TN 37831

evansb@ornl.gov

Fundamental knowledge of the molecular structural transitions that lignocellulosic biomass undergoes during processing is required to understand and improve its conversion to fuels. The capabilities of the Spallation Neutron Source (SNS), the High flux Isotope Reactor (HFIR), and the National Leadership Computing Facility (NCLF), all located at Oak Ridge National Laboratory, now enable the application of advanced neutron and computational techniques to this complex problem. We are developing and demonstrating an integrated technology that applies the power of neutron scattering and computer simulation supported by advanced NMR and chemical force microscopy to examine biomass structural changes during pretreatment. Each of the experimental techniques contributes complementary information that enables the visualization of lignocellulose and the effects of pretreatment. Understanding structural transitions of plant cell walls requires observation of morphology and association of the component biopolymers at nanometer to micrometer length scales. Small angle neutron scattering (SANS) provides structural information about morphology and molecular associations of biomass as well as enzyme structure. Deuterated enzymes, cellulose, and lignocellulosic biomass are being produced for SANS phase contrast experiments that will differentiate between components during biomass degradation. An in-situ reaction cell is being employed for imaging of biomass samples during pretreatment. Accurate interpretation of SANS data requires detailed chemical and physical characteristics of the samples as well as computer modeling of molecular conformation. Chemical and physical analyses, with NMR and X-ray diffraction (XRD) providing relevant details of chemical structure, chemical bonding, crystalline form, and crystallite sizes, provide this information. Chemical force and atomic force microscopy give complementary nanometer-scale surface characterization. Finally, computer simulation builds atomistic models of component biopolymers and lignocellulosic biomass based on the experimental information from the other methods. Concomitantly, the computer models assist in SANS analysis and experimental design. We have recently published the results of our studies on the structure of extracted loblolly pine lignin in solution and on lignin aggregation during dilute acid pretreatment of switchgrass.

HIGH THROUGHPUT TECHNOLOGY IN THE BIOENERGY AND BIOCHEMICALS FIELD

Nicole Labbé and Lindsey Kline

Center for Renewable Carbon
University of Tennessee
2506 Jacob Drive
Knoxville, TN 37996

nlabbe@utk.edu

There is a growing consensus that a biorefinery would be more economically viable by producing, in addition to biofuels, valuable co-products from the non-cellulosic fractions of lignocellulosic biomass such as lignin. This rapid change reevaluates lignocellulosic biomass, not as just an inexpensive source of carbohydrates, but as a source of three polymeric materials: cellulose, hemicelluloses and lignin that can be converted into products currently produced from crude oil. High throughput techniques to assess these biomass constituents from the field to the laboratory to the biorefinery has been investigated and developed. This presentation will demonstrate the important role infrared spectroscopy coupled with multivariate analysis could play in biomass development, production, selection and conversion for a biorefinery. In addition to determine the quality of biomass (chemical composition), the technique will also assist in the estimation of biomass performance (recalcitrant factors, ability to release sugars…).

SURFACE CHEMISTRY IN PROFILING BIOMASS CONVERSION

Orlando J. Rojas

Department of Forest Biomaterials
North Carolina State University
Raleigh, NC, 27695-8005, USA

ojrojas@ncsu.edu

A prerequisite to understanding the mechanisms involved in polysaccharide enzymatic reactions is the availability of measurement capabilities at the nano- and molecular scales. Common approaches to test enzyme activities on lignocellulosic substrates are bench-scale experiments. However, there is a need to obtain molecular insights about the interactions between enzymes, cellulose substrates and the products of bioconversion. In this presentation we will discuss a comprehensive bioanalytical platform that facilitates a better understanding of the mechanism and main variables that affect degradation of cellulose to simple oligomeric sugars. Validation of the proposed biosensing methods involves investigations of effects of molecular and chemical composition as well as conditions of use on the extent and dynamics of polysaccharide conversion. Main tools used in our approaches included quartz microgravimetry, surface plasmon resonance, AFM, XPS and MALDI-MS.

References: Analytical Chemistry 81: 1872 (2009); Langmuir 24:3880 (2008); Langmuir, 24: 11592 (2008)