Unlocking secrets to cheaper ethanol

Thursday, September 16, 2010

New research could help scientists identify the most effective pretreatment strategy and lower the cost of biomass conversion. Credit: Oak Ridge National Laboratory

New insight into the structure of switchgrass and poplars is fueling discussions that could result in more efficient methods to turn biomass into biofuel.

Researchers from the Department of Energy's Oak Ridge National Laboratory and Georgia Tech used small-angle neutron scattering to probe the structural impact of an acid pretreatment of lignocellulose from switchgrass. Pretreatment is an essential step to extract cellulose, which can through a series of enzymatic procedures be converted into sugars and then ethanol. The findings, published in *Biomacromolecules*, could help scientists identify the most effective pretreatment strategy and lower the cost of the biomass conversion process.

"My hope is that this paper and subsequent discussions about our observations will lead to a better understanding of the complex mechanisms of lignocellulose breakdown," said co-author Volker Urban of ORNL's Chemical Sciences Division.

A key finding is that native switchgrass that has been pretreated with hot dilute sulfuric acid undergoes significant morphological changes. While the data demonstrate that the switchgrass materials are very similar at length scales greater than 1,000 angstroms, the materials are profoundly different at shorter lengths.

Specifically, Urban and colleagues discovered that the diameter of the crystalline portion of a cellulose fibril increases from about 21 angstroms before treatment to 42 angstroms after treatment. Also, they learned that lignin concurrently undergoes a redistribution process and forms aggregates, or droplets, which are 300 angstroms to 400 angstroms in size.

"Our study suggests that hot dilute sulfuric acid pretreatment effectively decreases recalcitrance by making cellulose more accessible to enzymes through lignin redistribution and hemi-cellulose removal," Urban said. Recalcitrance refers to a plant's robustness, or natural defenses to being chemically dismantled.

Unfortunately, the apparent increase in cellulose microfibril diameter may indicate a cellulose re-annealing that would be counterproductive and may limit the efficiency of the dilute sulfuric acid pretreatment process, the researchers reported.

"Ultimately, the ability to extract meaningful structural information from different native and pretreated biomass samples will enable evaluation of various pretreatment protocols for cost-effective biofuels production," Urban said.

Small-angle neutron scattering measurements were performed at ORNL's High Flux Isotope Reactor and analyzed using the unified fit approach, a mathematic model that allows simultaneous evaluation of the different levels of hierarchical organization that are present in biomass.

Other authors of the paper were Sai Venkatesh Pingali, William Heller, Joseph McGaughey, Hugh O'Neill, Dean Myles and Barbara Evans of ORNL and Marcus Foston and Arthur Ragauskas of Georgia Tech. Support for the research and for HFIR was provided by DOE's Office of Science.

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