Biomass Studies: Growing Energy

Biomass research can help lower energy costs, reduce dependence on oil, and decrease pollution.

Biomass from plants offers a potentially abundant source of ethanol from the fermentation of component sugars. But its complex laminate structure, consisting of the biopolymers cellulose, xylan, pectin, and lignin often collectively termed lignocellulose is difficult to disrupt and break down into fermentable sugars. Pretreatment is required to separate the components, detach lignin, and discompose the cellulose fibers for efficient conversion to fermentable sugars.

To learn why lignocellulose is so difficult to break down, a team of ORNL researchers is using the Bio-SANS instrument at HFIR and the unique resources of the Cray XT4 supercomputer at the National Leadership Computing Facility (NLCF) at ORNL to investigate biomass samples from the BioEnergy Science Center (BESC), also at ORNL. Their goal is to visualize the breakdown of plant cell wall structures during biomass processing at length scales ranging from nanometers to microns.

This research project, "Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation," is high priority because DOE has targeted energy independence through cost-effective production of ethanol and other liquid fuels from renewable biomass as an important part of its mission. DOE says that achieving success in this project will benefit the broader goals of energy security, domestic economy, and pollution reduction. High-resolution visualization and characterization of biomass is also a key task outlined by the DOE's biomass for energy strategy. Researchers say that their current work will demonstrate the value of using an integrated neutron science and high-performance scientific computing method to solve real-world problems. A second important goal of the research is to develop molecular visualization techniques that can be extended to other fields, such as medical research; this goal would be difficult to achieve without the combined use of neutron scattering and high-performance computing.

Lignocellulosic biomass, the scientific term for plant leaves, stems, and roots, is an abundant and renewable resource. A wide range of potential sources exist, including stalks and leaves left after harvest; residues from the paper, pulp, and lumber industries; bioenergy crops such as switch grass hay and poplar trees; as well as municipal leaves and tree trimmings waste. Unfortunately, the processing required to break biomass down into fermentable sugars for alcohol production and creation of other products is more energy intensive and expensive than extracting starch from grains or pressing juice from sugar cane. The structure of plant cell walls, and how those walls are deconstructed or converted at the molecular level, is not fully understood.

Since biomass is a complex, multicomponent, and multiscale material, characterization techniques are required that span a range of length scales from angstroms to micrometers and that can differentiate between individual components in the native material. Neutron scattering and diffraction probe structures over this range of length scales and can provide a fundamental understanding of the structure at the atomic and molecular level. Neutrons are also excellent at "seeing" order in complex systems, which is also important for understanding why the plant cell wall and lignocellulose structures resist breakdown. The unprecedented detail of these studies of the structure of lignocellulose will help engineers develop new, cost-effective methods for breaking down lignocellulosic biomass and using it in the production

of fuels and chemicals. Neutrons are particularly good at locating where critical water molecules are. This is very important, since most of the reactions are hydrolysis, in which a polysaccharide is broken by adding water. In the future, the team will extend their work across a broader suite of instruments at SNS. This information will be complemented by chemical force microscopy, a technique in which nanometer-scale probes are modified with specific chemical groups to spatially map hydrogen bonding and hydrophobic interactions between lignocellulose components.

Computer simulation and modeling will integrate the neutron scattering data with information obtained from other complementary methods, thereby giving scientists a molecular-level understanding of the structure, dynamics, and degradation pathways of these materials. One computer-based method is a numerical simulation of biomolecular systems at the atomic level using a molecular dynamics (MD) approach, which involves the stepwise integration of the equations of motion of many-particle systems. This approach is limited by the restrictions of the available computer processing power and has therefore been applied to systems of at most ~105 particles and a 100-nanosecond timescale. The increased computer power now available at the NLCF allows extensions of the MD computer simulations to micrometer lengths and microsecond timescales, which allows the simulation of lignocellulosic biomass systems. Further extensions using coarse-grained mesoscale techniques will allow the simulation of even larger ensembles of heterogeneous biomass systems, thereby enabling numerical studies of the degradation process of the biopolymers in detail. The best-fit models of the lignocellulose molecules derived from their experimental neutron scattering profiles will then be compared to the results from these computer simulations, providing a combined experimental and theoretical picture of lignocellulosic biomass systems at the molecular scale.

In future work, the interplay between computer simulation and experiment will be enhanced by the development of codes for calculating the relevant neutron scattering structure factors directly from the simulation data; this will require the integration, automation, and optimization of standard biomolecular simulation programs for use in interpreting the results of neutron scattering from lignocellulosic targets. The team will then extend their studies to biological breakdown of biomass by microbes and enzymes, as well as to the growth and formation of cell walls in living plant cells. Our understanding of the behavior of water and of molecular order in these systems can clearly be greatly improved by the combined use of numerical studies using high performance computing and neutron scattering experiments on real biomass samples.

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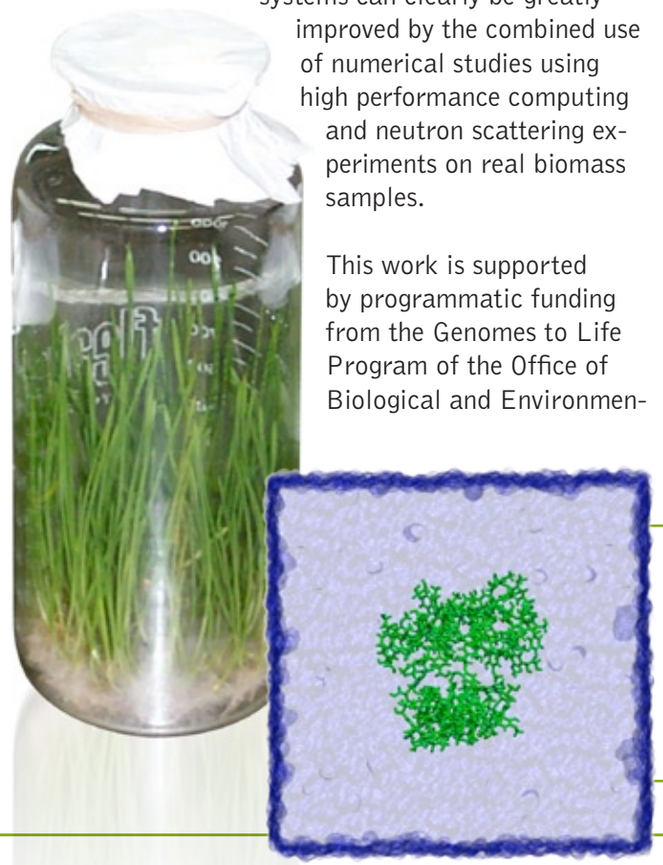
Research team:

- Barbara R. Evans and Joseph McGaughey, Chemical Sciences Division (CSD)
- Jeremy C. Smith and Loukas Petridis, Biosciences Division
- Volker Urban, William T. Heller, Hugh M. O'Neill, and Sai Venkatesh Pingali, Center for Structural Molecular Biology (CSMB) and CSD
- Dean A. Myles, Neutron Scattering Science Division
- Art Ragauskas, School of Chemistry and Biochemistry, Georgia Institute of Technology
- Ida Lee, Department of Electrical and Computer Engineering, University of Tennessee, Knoxville
- Brian Davison, Biosciences Division



Left: Biomass crops, such as the wheat shown here, are being grown in deuterated water mixtures to provide deuterated lignocellulosic material for neutron experiments. Right: The physical structure of lignin in aqueous solution was modeled using molecular dynamics-based computer simulation paired with scattering data.