186. Morphological Changes in the Cellulose and Lignin Components of Biomass Occur at Different Stages During Steam Pretreatment

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http://www.ornl.gov/science-discovery/clean-energy/research-areas/systems-biology/bioenergy/dynamic-visualization-of-lignocellulose

Project Goals: Lignocellulosic biomass comprises the vast majority of biomass on Earth and has the potential to play a major role in generation of renewable biofuels if cost-effective conversion can be achieved. Largely composed of plant cell walls, it is a complex biological composite material that is recalcitrant to the structural deconstruction and enzymatic hydrolysis into sugars that is necessary for fermentation to bioethanol. The Scientific Focus Area in Biofuels is developing "Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation" for multiple-length scale, real-time imaging of biomass during pretreatment and enzymatic hydrolysis. This is providing fundamental information about the structure and deconstruction of plant cell walls that is needed to drive improvements in the conversion of renewable lignocellulosic biomass to biofuels.

Understanding the structural changes in biomass during pretreatment is critical for increasing biomass conversion efficiencies. Currently biomass analysis techniques are limited to comparing biomass structure before and after pretreatment. However, it is extremely desirable to understand how the structure of lignocellulose changes during a pretreatment regime. Our previous work showed the formation of lignin globules and the aggregation of cellulose fibers in pretreated biomass. However, this work did not provide any insights into the processes that drive these structural changes. In order to address this knowledge gap we developed an approach to monitor morphological changes as they occur during steam explosion pretreatment (SEP) by placing a pressure reaction cell in a neutron beam and collecting time-resolved small-angle neutron scattering data.1 Changes to cellulose morphology occurred mainly in the heating phase of pretreatment, whereas changes in lignin morphology occurred mainly in the holding and cooling phases. During the heating stage, water is irreversibly expelled from cellulose macrofibrils as the elemental fibers coalesce. On the other hand, there is little change to lignin during the heating phase, but aggregates begin to appear and increase in number during the holding phase. Lignin aggregates continue to appear and increase in size during the cooling phase. These results support previous MD simulations that suggest that lignin aggregation occurs during SEP as soon as lignin has phase separated from hemicellulose.2 The results presented here indicate that this phase separation starts at ~140oC during SEP. This experiment demonstrates the unique information that in situ SANS studies of pretreatment can provide. This approach could be useful in optimizing the heating, holding and cooling stages of pretreatments to allow the exact size and nature of lignin aggregates to be controlled in order to enhance enzyme accessibility to cellulose and therefore the efficiency of biomass conversion.

References

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This research is funded by the Genomic Science Program, Office of Biological and Environmental Research, U.S. Department of Energy, under FWP ERKP752. The Center for Structural Molecular Biology (CSMB) and the Bio---SANS beam line is supported by the Office of Biological and Environmental Research, using facilities supported by the U. S. Department of Energy, managed by UT-Battelle, LLC under contract No. DE-AC05-00OR22725. This Research on Bio-SANS and GP-SANS at Oak Ridge National Laboratory's High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, Department of Energy.