Explaining and Predicting Biomass Recalcitrance with Rigidity Percolation Theory

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Project Goals: The BioEnergy Science Center (BESC) focuses on fundamental understanding and elimination of biomass recalcitrance. BESC's approach to improve accessibility to the sugars within biomass involves (1) improved plant cell walls for rapid deconstruction and (2) multi-talented microbes for converting plant biomass into biofuels in a single step [consolidated bioprocessing (CBP)]. Biomass research works with two potential bioenergy crops (switchgrass and *Populus)* to develop improved varieties and to understand cell wall biosynthesis pathways. We test large numbers of natural variants and generate specific modified plants samples. BESC's research in deconstruction and conversion targets CBP manipulating thermophilic anaerobes and their cellulolytic enzymes for improved conversion, yields, and titer. Enabling technologies in biomass characterization, 'omics, and modeling are used to understand chemical and structural changes within biomass and to provide insights into mechanisms.

There remains considerable debate on the roles, organization, and interactions of the various polymers within the plant cell wall and how each contributes to the cell wall recalcitrance. We present a model based on Rigidity Percolation theory demonstrating reduced recalcitrance is dependent on compositional variation of the major plant cell wall polymers, lignin, hemicellulose, pectin, and cellulose, from studies using natural variants and genetically-modified feedstocks. Rigidity percolation theory is a subset of general percolation theory that has been used in amorphous materials science to understand how compositional variation and the connectivity of the network structures affect physical properties. The theory was also evaluated over a range of feedstocks including alfalfa, switchgrass, eucalyptus, *Populus,* and pine. Rigidity percolation theory predicts a dramatic change in the physical properties of a system when the number of floppy modes with the network structure approaches zero. For the biomass samples studied here, the predicted change is observed when the plotting average coordination number versus sugar release indicating deconstruction mechanisms are more effective on plant cell walls composed of more floppy elements and hindered by more rigid elements.

This framework can also be used as a predictive tool to understand how changes in composition can influence biomass recalcitrance. Rigidity percolation theory can be used to predict alternate combinations of cell wall polymer composition that could produce low recalcitrant plant lines while supporting normal plant growth. The effective application of rigidity percolation theory will require moving beyond the current approach of modifying only individual cell wall polymers as a means of reducing recalcitrance.

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