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Multi-scale Structural Effects of Co-solvent Pretreatment of Lignocellulosic Biomass for Enhanced Biorefinery Efficiency

Efficient lignocellulosic biomass utilization is essential for sustainable biofuel and bioproduct manufacturing within a biorefinery framework. However, the inherent recalcitrance of plant cell walls - caused by densely packed cellulose fibrils embedded in a lignin-hemicellulose matrix - presents a significant obstacle to effective industrial-scale pretreatment. Therefore, cosolvent-pretreated biomass was characterized using small-angle neutron scattering (SANS) technique to determine structural parameters to predict the most efficient cosolvent pretreatment by combining with machine learning approaches. SANS was employed to probe the nanoscale structural evolution of solvent pretreated poplar biomass subjected to a comprehensive matrix of 163 experimental runs spanning three solvent severity levels (strong, medium, weak) and three varying pretreatment severities levels (2.07, 2.73, 2.95) based on temperature, residence time, and sulfuric acid concentration. Key structural parameters, including the radius of gyration (Rg), power-law exponent (P), and Guinier and Porod scalars (G, B) were extracted to quantitatively describe changes in size distribution of cellulose microfibril diameter, lignin/hemicellulose aggregate particle size, surface roughness of micron-sized structures like cell lumen. Statistical analysis revealed that solvent severity had a significant influence ($p = 0.05$) on smaller structural features, such as cellulose microfibril radius Rg, indicating that solvents strongly modulate biomass nanostructure, while pretreatment severity driven by sulfuric acid concentration and temperature did not result in statistically significant Rg difference, as well as increase in surface roughness. By establishing robust correlations between pretreatment conditions and nanoscale structural signatures, the study provides a predictive foundation for optimizing carbohydrate accessibility and yield using the cutting-edge SANS technology combined with advancing biorefinery technologies.

Topical Area

Soft matter: polymers, and complex fluids

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