Mathematical Modeling and Simulation of Biofuel Production from Lignocellulosic Biomass

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Renewable energy or biofuel from lignocellulosic biomass is an alternative way to replace the depleting fossil fuels. The production cost can be reduced by increasing the concentration of biomass particles. However, lignocellulosic biomass is a suspension of natural fibers, and processing at high solids concentration is a challenging task because it will affect the mixing quality between enzyme and cellulose particles, and the generation of sugars. Thus, understanding the factors that affect the rheology of the biomass suspension is crucial in order to maximize the production at minimum cost. Our aim is to develop a solution strategy for the modeling and simulation of high solid concentration of biomass suspension during enzymatic hydrolysis. Also, we intend to develop a multi-scale model for enzymatic hydrolysis that captures the reaction kinetics of cellulose chains in PBE form, cellulose rod orientation and interaction, as well as hydrodynamics and plasticity of the biomass mixture. We extended and improved the established kinetic model proposed by Griggs et al. We built the reduced order models by ignoring significantly small term and determined the approximate solutions by employing asymptotic analysis method. Liquid crystal theory is adopted to study the cellulose fibers. The complete model is solved using DAE-QMOM technique in finite-element software package, COMSOL. Essentially, we made a clear connection between microscopic, mesoscopic, and macroscopic properties of biomass slurries undergoing enzymatic hydrolysis. The results show that the quality of mixing within a reactor is crucial in optimizing the hydrolysis product. Also, the biomass suspension shows non-Newtonian behaviors such as shear thinning, yield stress, and normal stress difference which is an agreement with experimental results. The extended model improved the predictive capabilities, hence increased our understanding of the behavior of biomass suspension.