A Diffusion and Surface Reaction Model for Highlighting Key Factors in the Enzymatic Hydrolysis of Lignocellulosic Biomass

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Efficient enzymatic hydrolysis of lignocellulosic biomass is essential to the cost effective production of fuels and chemicals from plants. However, due to the intricate nature of the substrates and the broad diversity of biomass and enzymes systems, an in-depth understanding of the key aspects governing this process, coming from both theoretical and experimental ends, is still lacking. While several factors, such as cellulose accessibility and unspecific adsorption of enzymes on the protective lignin barrier, have been suggested as major bottlenecks in the digestion process, a quantitative study assessing the relative importance of these mechanisms has yet to be done.

In the present study, we developed a flexible, comprehensive model of the enzymatic hydrolysis of lignocellulosic materials based on pore-diffusion and surface reactions. Relying on the initial composition and pore size distribution of the lignocellulosic substrate, predictions properly captured initial hydrolysis rates when compared to available data in literature. However, in contrast to the usual slowdown observed in the reaction rate for common enzyme loadings, computed yields showed no development of hindrance as the reaction proceeds. By correlating the enzyme loading in terms of accessible surface to the rate of glucose release, the model can not only shed light on the origin of this apparent decrease – heterogeneity in cellulose digestibility, enzyme deactivation pathways –, but also on the enzyme synergism regarding the surface accessibility. In this perspective, current work focuses on evaluating the implications of enzyme loadings on the hydrolysis rate of acid pretreated beech wood by comparing *in silico* results with experimental observations. The ultimate goal of our work is to facilitate the rational design of biomass processing and engineered cellulase cocktails.