

Abstract Submitted
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A coupled CFD and two-phase substrate kinetic model for enzymatic hydrolysis of lignocellulose¹ NICHOLAS DANES², Colorado Sch of Mines, HARISWARAN SITARAMAN, JONATHAN STICKEL, MICHAEL SPRAGUE, National Renewable Energy Lab — Cost-effective production of fuels from lignocellulosic biomass is an important subject of research in order to meet the world's current and future energy demands. Enzymatic hydrolysis is one of the several steps in the biochemical conversion of biomass into fuels. This process involves the interplay of non-Newtonian fluid dynamics that happen over tens of seconds coupled with chemical reactions that happen over several hours. In this work, we present a coupled CFD-reaction model for conversion of cellulose to sugars in a benchtop mixer reactor. A subcycling approach is used to circumvent the large time scale disparity between fluid dynamics and reactions. We will present a validation study of our simulations with experiments for well-mixed and stratified reactor scenarios along with predictions for conversion rates and product concentrations at varying impeller speeds and in scaled-up reactors.

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