Investigation of Mixing Issues in Enzymatic Hydrolysis of Lignocellulosic Biomasses for Bioethanol Production via CFD and Experiments

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Abstract

Second generation biofuels are produced sustainably by using biomasses consisting of the residual non-food parts of current crops that are left behind once the food crop has been extracted, partially addressing the "food or fuel" dilemma. Although the technology seems promising a number of issues need to be addressed, including the improvement of biotechnological aspects, the design of novel and efficient mixing equipments as well as their scale up to continuous industrial processes. This work focuses on the investigation of enzymatic hydrolysis of lignocellulosic biomasses, that together with fermentation represents the key step of the bioethanol production process. Many of the relevant mixing issues, related for example to the contact between the biomass and the enzyme, can be addressed through mathematical modeling, if a reliable rheological model of the pretreated biomass is provided. The lignocellulosic slurry (processed during hydrolysis) presents a non-Newtonian behavior, of viscoplastic type, which is very difficult to characterize with standard rheological measurements. To overcome this problem, in this work computational fluid dynamics (CFD) is used in combination with experiments, carried out on a laboratory scale anchor rector, to identify rheological parameters by employing two different approaches, namely the power law and the Herschel-Bulkley models. The methodology was firstly validated by using fluids with known rheological behavior (i.e., aqueous solutions glycerol and of guar gum) and was then applied to our test material: arundo pretreated by steam explosion. Three-dimensional CFD simulations and experiments on the anchor rector were carried out under different arundo concentrations (18 - 35% w/w), stirring velocity (12 – 200 rpm) and hydrolysis time (0 - 4 hr.). The CFD simulations were carried out by using the moving reference frame approach; great care was used in the development of the computational grid and in the solution of numerical issues. The validation of the method via comparison with the experiments with glycerol and guar gum resulted in very close agreement. The identification of the rheological parameters for the pretreated biomass (and their time evolution during hydrolysis) was successful and resulted in good agreement with the literature. These results were subsequently used to test different laboratory- and pilot-scale impeller reactors. The CFD model is currently being used to design an industrial continuous reactor for enzymatic hydrolysis and is being extended to model fermentation. Our future work will focus on the use of the CFD model to develop a continuous simultaneous hydrolysis/fermentation process.

keywords: computational fluid dynamics, non-Newtonian fluids, bioethanol, enzymatic hydrolysis, identification of rheological models

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