Kinetics modeling for design of continuous enzymatic hydrolysis

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Background

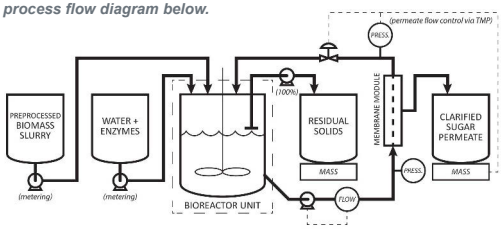
- Design of advanced enzymatic hydrolysis (EH) reactor concepts such as continuous EH are complicated by a lack of applicable, computationally accessible models
- EH models generally fall into two categories: fundamental mechanistic models which elucidate the mechanisms of deconstruction but are computationally expensive, and batch reactor models which require knowledge of the substrate's reaction-history. However, neither of these model types is suitable for application in novel process or reactor design concepts
- Phenomenological models focused on the relevant phenomena may bridge the gap and provide reasonable fidelity for novel contexts

Batch Experiments

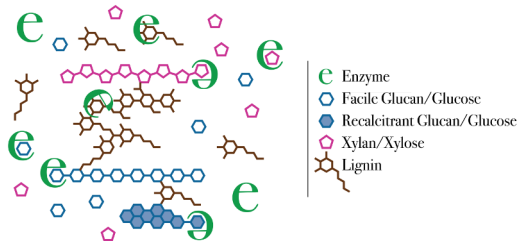
- Data from a series of batch experiments were used to find best-fit model parameters
- De-acetylated (0.4% wt NaOH, 80°C, 2h) and dilute-acid pretreated (1.0% wt, 160°C, 15 min) (DDA) corn stover was used across all experiments
- Base conditions of 10% insoluble solids mass fraction (f_{is}), 20 mg/g CTEC3 (Novozymes)
- Additional runs included dosed sugars, decreased enzyme loading, and varied initial solids to probe the parameter space

Continuous EH Experimental Setup

Continuous EH apparatus consisted of a vertically-stirred tank vessel with a pump-around-loop nanofilter (100 kDa MWCO) to remove liquors, with pretreated solids and buffer fed into the reactor, and a purge stream removing spent slurry. Pictured above, with a process flow diagram below.



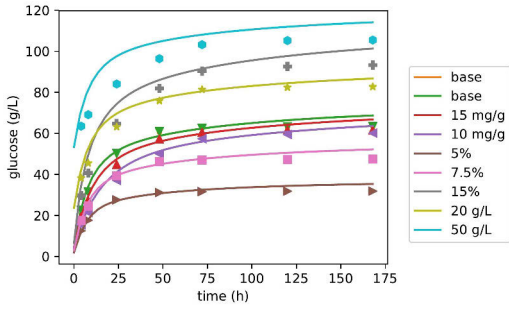
Model Formulation

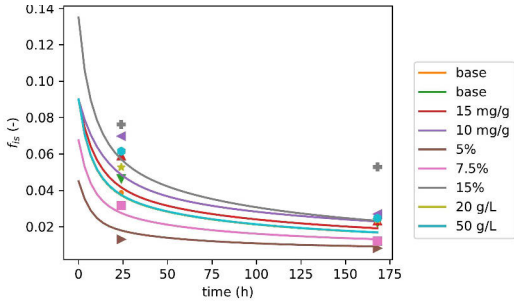


Key assumptions:

- Enzyme is modeled as a single generic population
- Cellulose is partitioned into facile and recalcitrant populations (two-phase substrate model). These share the same kinetic rate, but the facile population is fully accessible (high adsorption) while the recalcitrant population has structure which limits its availability (lower adsorption
- Lignin is solubilized during EH
- Biomass is otherwise modeled without structure
- Enzyme is inhibited by lignin (soluble as well as solid), and by soluble sugars
- Enzyme deactivation is negligible, i.e., **not** a significant driver of rate slowdown

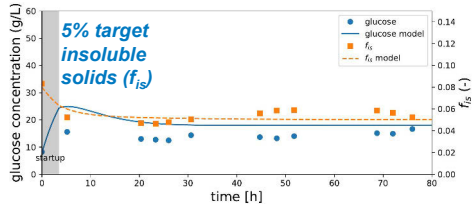
Model Fit to Batch EH

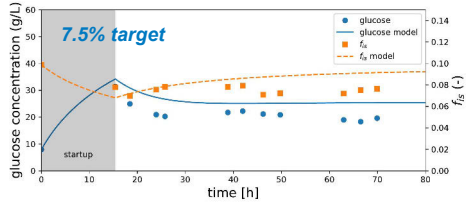


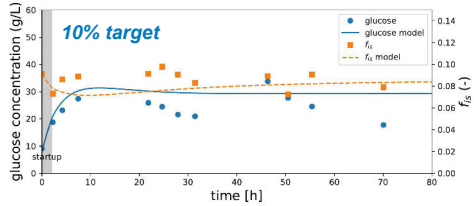


The model was fit with reasonable fidelity to our batch data.

Application to Continuous EH Data

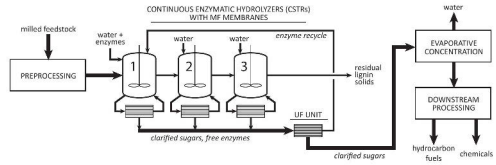






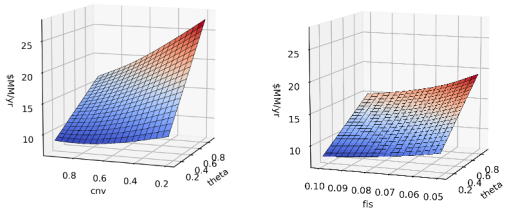
The model produced using batch data shows good agreement with continuous EH results

Techno-Economic Sensitivities



fis = 7.5%

cnv = 95.0%



A lightweight model implemented in ASPEN+ allows us to examine sensitivities in process design and understand tradeoffs imposed by reaction fundamentals. Increasing targeted conversion, limiting water use and thus membrane costs (theta), and increasing insoluble solids fraction improve the economics.

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