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ENZYMATIC CATALYSIS OF BUTYL LEVULINATE SYNTHESIS IN CONTINUOUS MICROFLUIDIC SYSTEM: KINETIC MODEL ASSESSMENT

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PURPOSE OF THE ABSTRACT

Nowadays, biomass valorization has attracted great interests as its products have shown potential to substitute the fossil-oriented products. Conversion of biomass to biofuels, materials and chemicals is of great interest in chemical engineering. [1] Levulinic acid (LA) is obtained from lignocellulosic biomass and it has been defined as one of the 12 most promising building blocks. [2] Esterification of this platform molecule leads to the production of alkyl levulinates, used mainly as solvents, additives and as biofuels. In fact, these are utilized as starting molecules for the production of other high-added value chemicals, such as gamma valerolactone.[3]
In this study, we have assessed different kinetic model for the esterification of LA by butanol over immobilized enzyme in microfluidic reactor. The first part includes a series of experiments conducted in a microfluidic reactor in which Novozymes 435 (immobilized) [4] was packed. The use of a microfluidic reactor allows to decrease concentration and thermal gradients, and hence plug-flow model can be used. The second part of this study is focused on the development and assessment of kinetic models based on experiments. Modelling was done by Athena Visual Studio® software, using a Bayesian framework. [5]
Experiments were performed using levulinic acid, 1-butanol and Novozyme 435 in a microfluidic reactor. The reactor is equipped with a syringe pump, which is used to inject the reactants in the microfluidic reactor, an omnifit column, in which the enzymes were immobilized, and a system to collect the mixture for subsequent analyzes. GC was used to identify and quantify the composition of the reaction mixture.

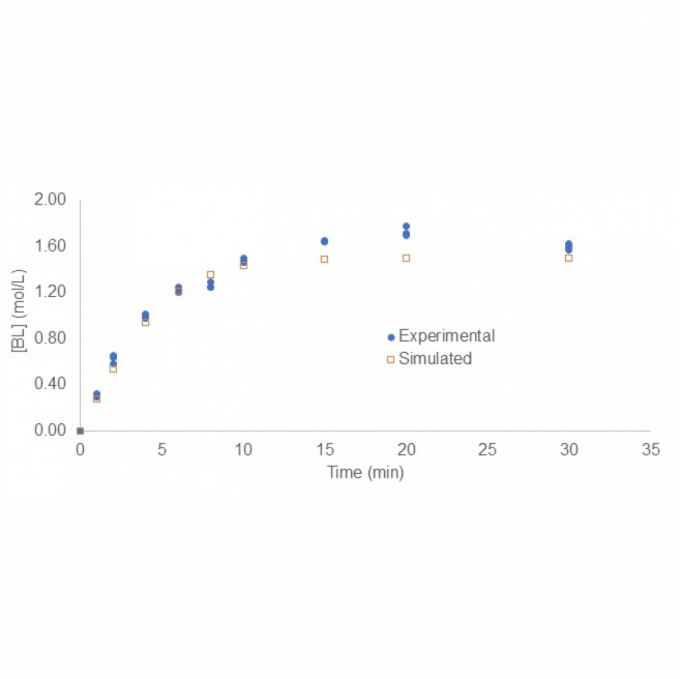
Residence time distribution study showed that internal and external mass transfer can be neglected. Deactivation of enzyme was found to be negligible for 10 hours. For the kinetic study, different conditions such as substrate concentration, catalyst loading, and temperature were applied to the esterification of levulinic acid by butanol. A Ping-Pong Bi-Bi mechanism with alcohol inhibition was found to be the most adequate.[6] Figs 1 and 2 show the fit of the model to one experiment.

Figure 1. Fit of model to the experimental concentration of BL at 65°C and [LA]inlet=2.61 mol/L.

Figure 1. Fit of model to the experimental concentration of BL at 50°C and [LA]inlet=5.16 mol/L.

The combination of biocatalysis and flow chemistry opens powerful new process windows, indeed, enzymatic catalysis has many benefits such as mild operation conditions, high product specificity and low pollution. [7] We have been able to describe the enzymatic mechanism by developing an original method, assessed by Bayesian inference.

FIGURES



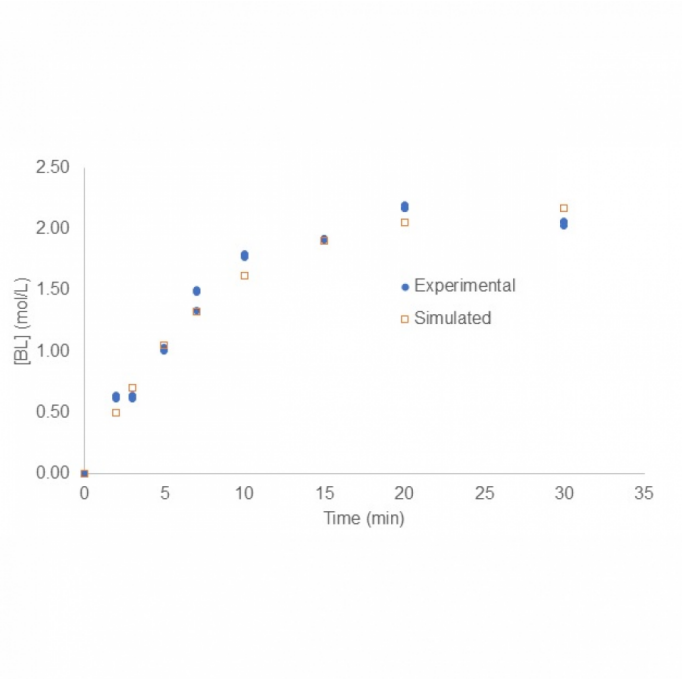


FIGURE 1

Figure 1

Figure 1. Fit of model to the experimental concentration of BL at 65°C and [LA]inlet=2.61 mol/L.

FIGURE 2

Figure 2

Figure 1. Fit of model to the experimental concentration of BL at 50°C and [LA]inlet=5.16 mol/L.

KEYWORDS

biocatalysis | microfluidic | kinetics | bayesian statistics

BIBLIOGRAPHY