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SIMULATION OF ENZYMATIC HYDROLYSIS OF WHEAT STRAW USING AUTOHYDROLYSIS AND ORGANOSOLV PROCESSES

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Simulation, modeling, enzymatic hydrolysis..

ABSTRACT

The modeling and simulation of enzymatic hydrolysis pretreated solids obtained by a sequence of autohydrolysis (solubilization of hemicellulose) and organosolv (solubilization of lignin) were studied. Two kinetic models for glucose production were compared and its kinetic constants calculated. According to the obtained results, enzymatic saccharification of the autohydrolysis pretreated solids (APS) proved to be more effective than when the organosolv pretreated solids (OPS) were used. The maximum extent of the enzymatic conversion of cellulose to glucose was 90.88 % and 64.04 %, for APS and OPS respectively, at 96 h. Models based on first and second order cellulase deactivation kinetics satisfactory predicted the behavior of glucose production..

METHODOLOGY

For the remaining pages follow the general guidelines below:

Enzymatic hydrolysis

The autohydrolysis (APS) and sequence of autohydrolysis and organosolv (OPS) pretreated solids were used as substrate for enzymatic saccharification.

Enzymatic saccharification were performed in a jacketed glass reactor with a working volume of 50 mL (total volume of 75 mL) at 50 ºC by duplicate, using cellulase (Celluclast 1.5 L) and β-glucosidase (Novozyme 188) with a loading of 40 FPU/g and 60 IU/g of cellulose, respectively, in 50 mM citrate buffer (pH 4.8) with 2 % (w/v) sodium azide to inhibit microbial contamination and a final cellulose concentration of 1 % (w/v).

The necessary amount of deionized water was calculated and added to make the total volume of 50 mL. Novozyme 188 was supplemented in order to eliminate the inhibition effect of cellobiose. Agitation was carried out using a magnetic stirrer (150 rpm) and samples were taken at 3 h intervals for the first 12 h and at 24 h intervals until a total time of 96 h. The samples were kept in boiling water for 5 min to inactive enzymatic activity, and then centrifuged at 8260 x g for 10 min to remove insoluble substrate; the supernatant was filtered through a 0.2 µm sterile membrane filter analyzed for soluble sugars in HPLC.

Modeling and simulation of enzymatic hydrolysis

Cellulase consists of three components is assumed to form a single combined effect on the hydrolysis of insoluble substrate. The assumptions of the model are: 1) cellulase enzyme containing endo-β-1,4-glucanase, exo-β-1,4-cellobiohydrolase and assuming a single combined effect in the hydrolysis of insoluble substrate; 2) surface structure of insoluble substrate was considered homogeneous. It is shown as the following equation.

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P \qquad (1)$$

Applying mass action law and quasi-steady-state theory, a mathematical equation cab be deduced as follow:

$$[p] = [S_0]\left[1 - exp\left(-k_2 \int_0^t \frac{[E]}{K_e + [E]dt}\right)\right] \qquad (2)$$

where Ke is the equilibrium constant. [S0], [*p*] and [*E*] represent concentrations of initial substrate, product and enzyme. When cellulase deactivation is considered as a first order reaction, the deactivation rate can be expressed by:

$$\frac{d[E]}{dt} = -k_{de1}[E] \tag{3}$$

When cellulase deactivation is considered as a second order reaction, the deactivation rate can be expressed by the following equation:

$$\frac{d[E]}{dt} = -k_{de2}[E^2] \tag{4}$$

The simulation of first and second order model was performed using Matlab software.

RESULTS AND DISCUSSIONS

Simulation of first and second order model

The experimental glucose data concentration profiles of the enzymatic hydrolysis of APS and OPS, were fitted corresponding to the first and second order kinetic models, are shown in the Fig. 1A-B. In all cases, a good agreement with the experimental results was obtained (correlation coefficient, $R^2 > 0.97$).

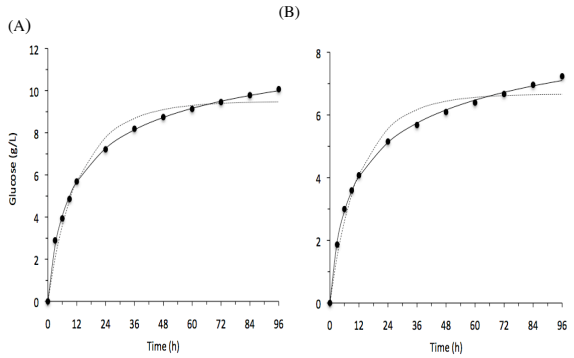

Figure 1. Simulation modeling for glucose concentration by enzymatic hydrolysis. (A) APS; (B) OPS; modeling based on 1st order reaction (····); modeling based on 2nd order reaction (—).

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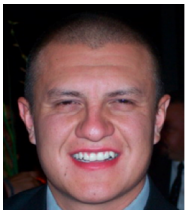

HECTOR RUIZ was born in in Saltillo, Coahuila Mexico and went to Autonomous University of Coahuila, where he studied chemical engineering and obtained his degree in 2004. He worked for three years for Peñoles Chemical Company before moving in 2007 to the University of Minho where he is studying his PhD in Chemical and Biological Engineering.