Supplementary Materials

Kinetic Characterization of Enzymatic Hydrolysis of Apple Pomace as Feedstock for a Sugar-based Biorefinery

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The substrate concentration S was assessed as follows from the experimental data at any time as the difference between the initial glucan concentration (S_0) and the glucose concentration (P).
The assessment of V_{Max}, K_M parameters was carried out by regression of data from short-term hydrolysis tests (1 h) through Equations (1) and (3) using Matlab® codes.
The assessment of the K_i parameter in the Michaelis and Menten model was carried out by the regression of glucose concentration data at any time from long-term hydrolysis tests (72 h) according to the mass balance on glucose in the hydrolysis liquid volume (Equations (A1)–(A3)).

$$\frac{dP}{dt} = V(S) \quad \text{(A1)}$$

$$P(t = 0) = 0 \quad \text{(A2)}$$

$$S = S_0 - P \quad \text{(A3)}$$

$V(S)$ was replaced in Equation A1 by RHS term of Equation 2. Data regression was performed in order to obtain the best fitting value of the parameter K_i by fixing the values of parameters V_{Max} and K_M at those obtained from short term hydrolysis data regression and fixing the enzyme concentration at the concentration adopted in the long-term tests.
The assessment of the k and n parameters in Chrastil's model was carried out by the regression of glucose concentration data at any time from long-term hydrolysis tests (72 h) according to the glucose concentration time course in Equation (3), by calculating P according to Equation A3 and fixing P_∞ at the value corresponding to the maximum experimental concentration of glucose for each data set.
All the data regressions were performed by using Matlab® codes. In particular, the codes used for the assessment of kinetic parameters from data of long-term hydrolysis tests were developed according to Andreozzi et al. (2006). The used optimization method allowed the assessment of the unknown kinetic parameters by simultaneous minimization of the standard deviation between the calculated and the experimental data for the three sets at different initial substrate concentrations S_0.

References

S1) Andreozzi, R., Caprio, V., Di Somma, I., Sanchirico, R. 'Kinetic and safety assessment for salicylic acid nitration by nitric acid/acetic acid system' Journal of Hazardous Materials (2006) 134 (1-3), 1-7