Electronic Supplementary Material (ESI) for RSC Advances

The Kinetics of Brønsted Acid-Catalyzed Hydrolysis of Hemicellulose Dissolved in 1-Ethyl-3-Methyl Imidazolium Chloride

Kristopher R. Enslow[1,2] and Alexis T. Bell[1,2]*
[1]*University of California, Berkeley, California 94720-1462*
[2]*Energy Biosciences Institute, Calvin Laboratory, Berkeley, California 94720-1462*
*alexbell@cchem.berkeley.edu

Supplemental Information

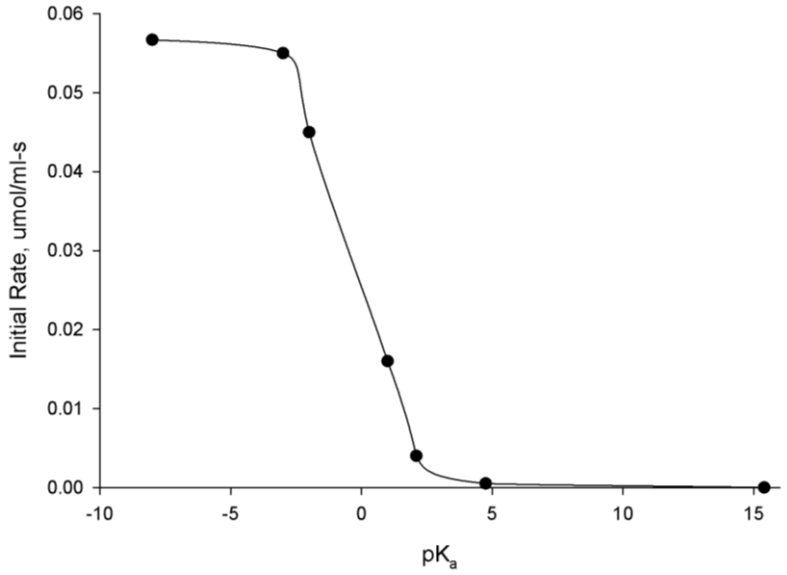

Figure A. Initial rate of xylan hydrolyis at 80 ºC in [Emim][Cl] catalyzed by various acids (200 mM) with 1.8 M water. Acids used: HCl (pKa = -8), H_2SO_4 (pKa = -3), CH_3SO_3H (pKa = -2), CF_3COOH (pKa = 1), H_3PO_4 (pKa = 2.1), CH_3COOH (pKa = 4.75), and H_2O (pKa = 15.4).

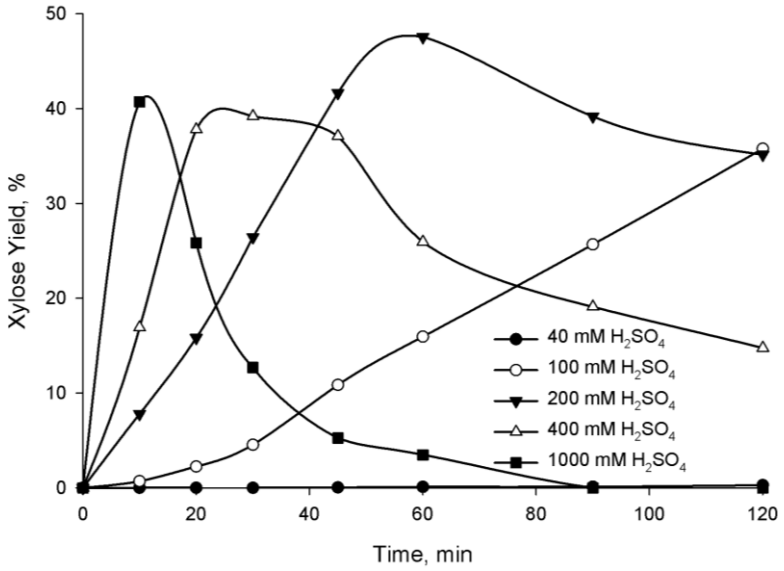

Figure B. Effect of H_2SO_4 concentration on xylose yield from xylan hydrolysis at 80 ºC in [Emim][Cl]. Concentrations used: 40 mM, 100 mM, 200 mM, 400 mM, and 1000 mM.

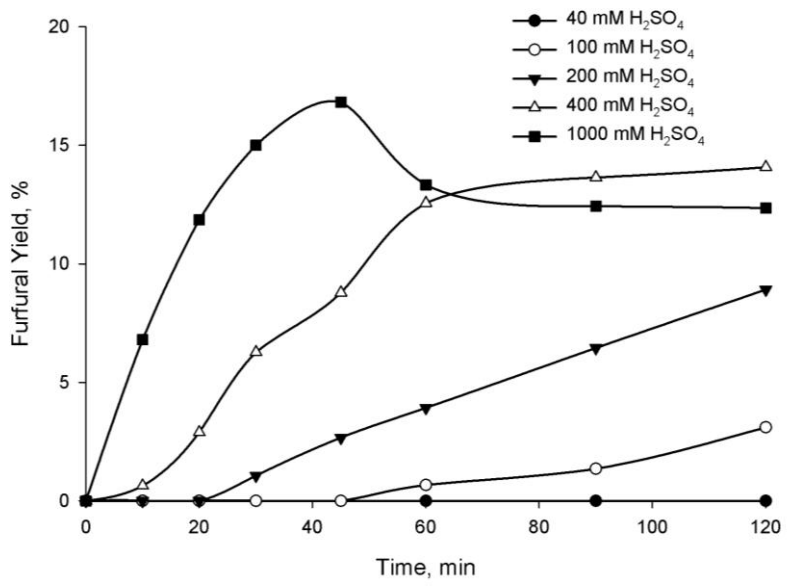

Figure C. Effect of H_2SO_4 concentration on furfural yield from the dehydration of xylose from xylan hydrolysis at 80 ºC in [Emim][Cl]. Concentrations used: 40 mM, 100 mM, 200 mM, 400 mM, and 1000 mM.

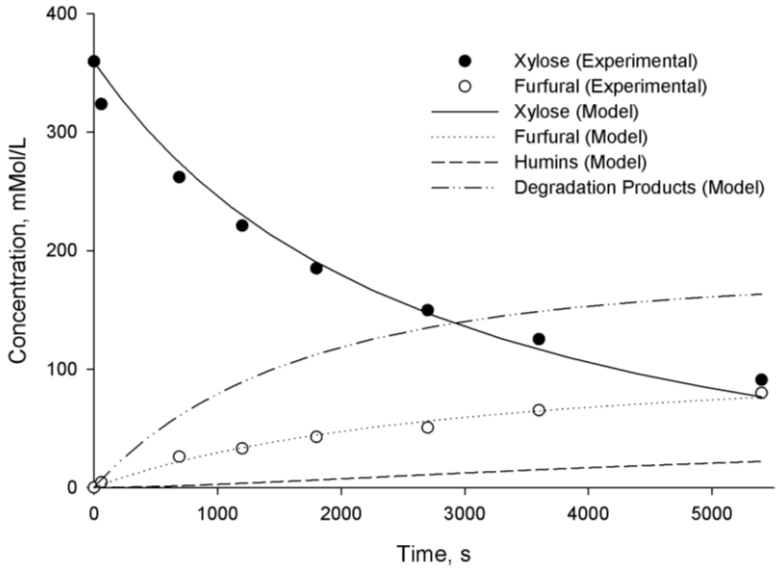

Figure D. Kinetic model fit to the experimental data from Figure 2 (for xylose dehydration), determined by least squares minimization of residuals using the lsqcurvefit and ode45 routines within MATLAB (R2010b). Figure shows the predicted xylose dehydration/degradation and the yields of furfural, humins, and degradation products over time.

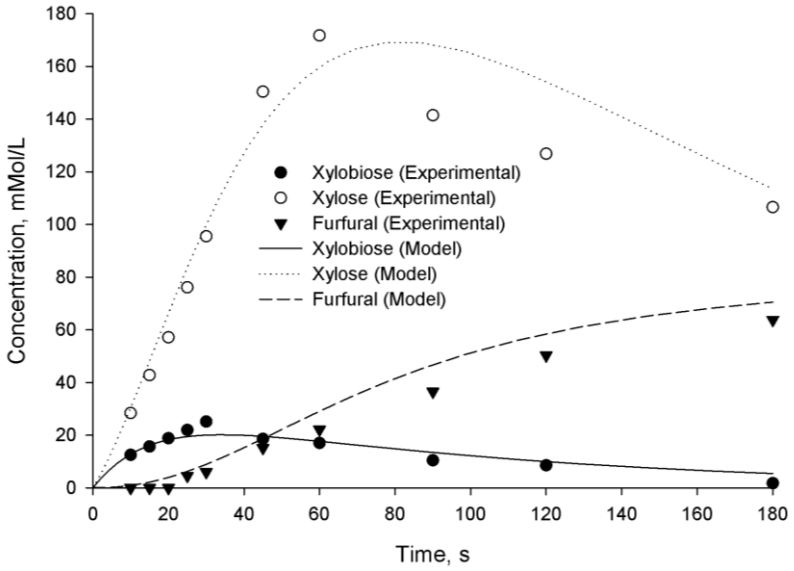

Figure E. Kinetic model fit to the experimental data from Figure 1 (for xylan hydrolysis), determined by least squares minimization of residuals using the lsqcurvefit and ode45 routines within MATLAB (R2010b). Figure shows the predicted yields of xylobiose, xylose, and furfural over time from the hydrolysis of xylan.

	Xylobiose	Xylose	Furfural[d]	Humins
No Dioxane	3%	38%	13%	10%
1:1 v/v Dioxane/IL[a]	4%	42%	7%	0%
30 min Extractions[b]	4%	43%	6%	0%
15 min Extractions[c]	5%	44%	5%	0%

Table A. The effect of using 1,4-dioxane on the production of humins created through xylan hydrolysis. Reaction conditions: 80 ºC, 90 minutes, 200 mM H_2SO_4, 1.8 M H_2O, 27 mg xylan, 500 ul [Emim][Cl]. [a]500 ul 1,4-dioxane used. [b]500 ul 1,4-dioxane used, extracted and replaced at 30 minute intervals (3 total extractions). [c]500 ul 1,4-dioxane used, extracted and replaced at 15 minute intervals (6 total extractions). [d]Furfural yield represents the sum of furfural detected in the [Emim][Cl] phase and all 1,4-dioxane phases.