

Fuzzy-enhanced modeling of lignocellulosic biomass enzymatic saccharification

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Supplementary Material

Table 1. Data Sets Carbohydrates Concentration - Value $\pm$ Standard Error

Fitting Data Sets										Validation Data Sets			
Data Set 1 – High Solids Batch					Data Set 2 – Low Solids Fed-Batch				Data Set 3 – Mixed Profile Fed-Batch				
Time (h)	Glucose (g.L ⁻¹)		Xylose (g.L ⁻¹)		Glucose (g.L ⁻¹)		Xylose (g.L ⁻¹)		Glucose (g.L ⁻¹)		Xylose (g.L ⁻¹)		
	Replicate		Replicate		Replicate		Replicate		Replicate		Replicate		
	1	2	1	2	1	2	1	2	1	2	1	2	
0.0	5.44	6.01	5.99	8.32	6.75	7.31	0.57	6.80	5.66	5.66	4.54	4.54	
0.5	6.38	6.77	6.17	8.61	8.69	9.20	2.85	7.72	7.92	7.80	5.49	5.58	
1.0	11.47	10.65	7.40	8.98	10.74	11.40	3.29	8.13	13.20	12.24	8.17	8.17	
2.0	11.60	12.21	8.42	9.15	13.83	13.00	8.71	8.60	17.16	16.26	10.02	10.02	
4.0	15.22	16.05	9.93	11.09	18.97	20.16	10.40	11.77	21.84	21.02	12.22	12.22	
6.0	19.04	19.76	11.53	12.61	22.03	23.25	11.08	12.81	25.92	24.41	12.89	12.89	
8.0	21.70	22.06	13.36	13.70	24.61	25.94	11.62	13.55	27.12	26.11	13.54	13.54	
12.0	26.62	26.20	14.31	15.27	28.08	28.63	12.75	14.35	30.24	29.10	14.35	14.35	
24.0	30.06	31.43	16.31	17.55	35.11	36.85	14.99	17.21	35.88	35.47	16.59	17.20	
36.0	33.85	35.39	17.51	18.94	38.75	40.66	16.86	18.84	39.60	38.94	17.41	18.84	
48.0	35.39	37.00	17.87	19.48	41.80	43.56	17.59	19.73	41.64	40.91	18.09	19.72	
60.0	35.83	37.46	17.83	19.43	44.06	45.62	18.64	20.29	42.48	42.07	18.64	18.64	
72.0	37.85	39.57	18.66	19.50	45.44	47.23	19.35	20.73	43.56	43.56	18.79	18.80	
96.0	37.84	39.56	18.95	19.94	47.47	48.24	19.00	21.52	44.88	45.43	19.85	19.85	

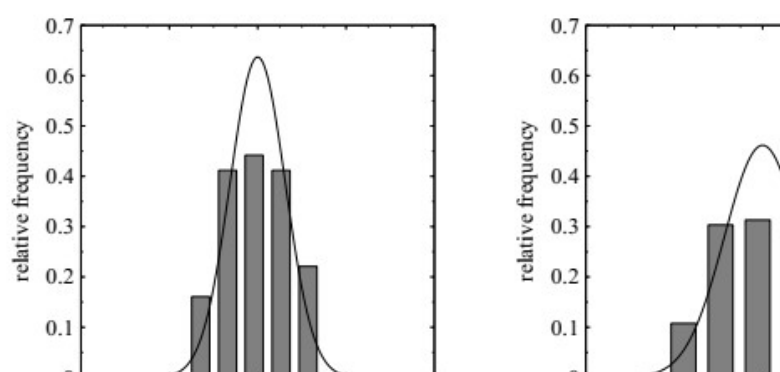


Figure 1. FM Error distribution between data sets replicates.

Table 2. High and Low Heterogeneous Michaelis-Menten Model Parameters for 6 Reactions System – Parameter $\pm$ Standard Error

Reaction	Solids Model	Parameters			
		k (min ⁻¹)	K _m (g.L ⁻¹)	K _p (g.L ⁻¹)	k _e (min ⁻¹)
1	High	$(1.01 \pm 9.57) \cdot 10^{-3}$	$(4.96 \pm 2.11) \cdot 10^{-2}$	$(6.06 \pm 4.22) \cdot 10^{-6}$	-
	Low	$(0.51 \pm 1.70) \cdot 10^{-2}$	$(0.50 \pm 2.31) \cdot 10^{-6}$	$(1.60 \pm 1.03) \cdot 10^{-4}$	-
2	High	$(1.24 \pm 2.91) \cdot 10^{-3}$	$(7.74 \pm 5.38) \cdot 10^{-3}$	$(0.49 \pm 2.14) \cdot 10^{-1}$	-
	Low	$(4.60 \pm 6.47) \cdot 10^{-4}$	$(0.31 \pm 1.48) \cdot 10^{-2}$	$(1.62 \pm 0.00) \cdot 10^{-2}$	-
3	High	$(3.93 \pm 6.53) \cdot 10^{-2}$	$(5.06 \pm 0.12) \cdot 10^{-4}$	$(0.93 \pm 3.32) \cdot 10^{-1}$	-
	Low	$(5.41 \pm 2.68) \cdot 10^{-2}$	$(0.10 \pm 3.58) \cdot 10^{-9}$	$(2.27 \pm 0.00) \cdot 10^{-1}$	-
4	High	$(2.11 \pm 1.29) \cdot 10^{-3}$	$(2.76 \pm 0.73) \cdot 10^{-2}$	$(1.80 \pm 1.25) \cdot 10^{-1}$	-
	Low	$(3.11 \pm 0.69) \cdot 10^{-3}$	$(7.13 \pm 0.16) \cdot 10^{-2}$	$(1.17 \pm 0.01) \cdot 10^{-1}$	-
6	High	-	-	-	$(8.43 \pm 2.09) \cdot 10^{-1}$
	Low	-	-	-	$(1.06 \pm 0.01) \cdot 10^{-1}$

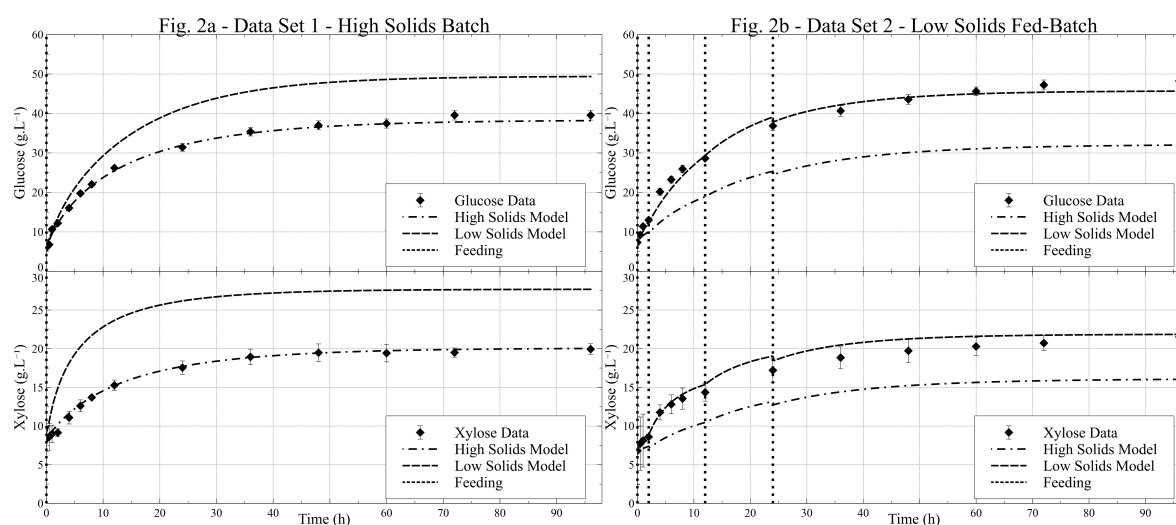


Figure 2. High Solids Model and Low Solids Model Fitting for 6 Reactions System – Fig. 2a Models prediction for Data Set 1; Fig. 2b Models prediction for Data Set 2; Error bars in data points are the

assay standard error for the compound concentration; Vertical dotted lines are the solids feeding times.

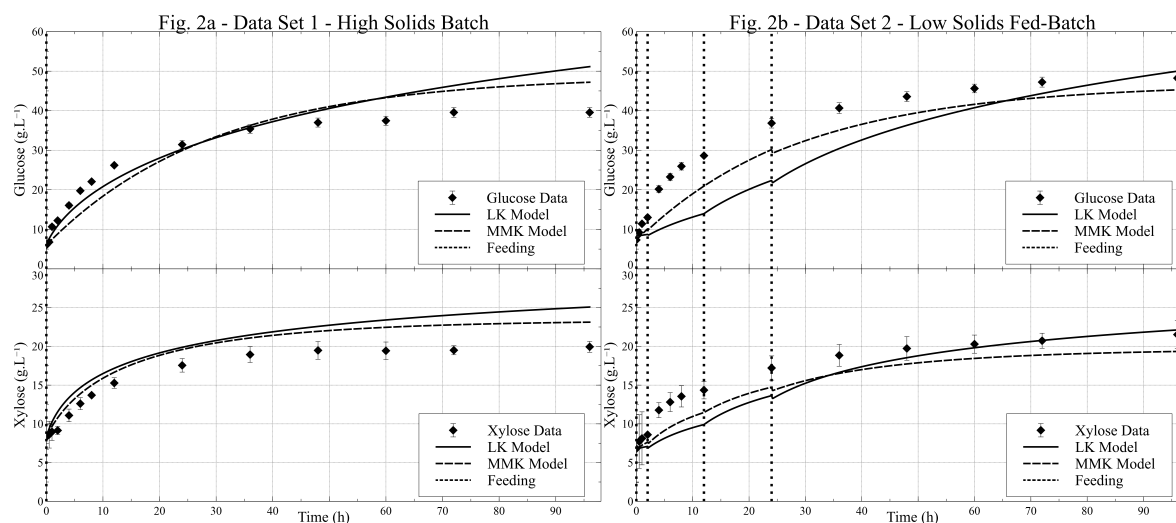


Figure 3. Langmuir Type Kinetics (LK) and Michaelis-Menten Kinetics (MMK) Fitting for 5 Reactions System – Fig. 3a Models prediction for Data Set 1; Fig. 3b Models prediction Data Set 2; Error bars in data points are the assay standard error for the compound concentration; Vertical dotted lines are the solids feeding times.



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