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SUPPORTING INFORMATION

Transforming biomass conversion with ionic liquids: process intensification and the development of a high-gravity, one-pot process for the production of cellulosic ethanol

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Table S1. Process and economic data for the three scenarios studied in the TEA

	Water-wash ^a	One-pot HG (current) ^b	One-pot HG (projected) ^c
Biomass processed (dry MT/day)	2000	2000	2000
Biomass price (\$/dry ton, delivered at plant-gate)	80	80	80
Pretreatment			
IL used	[C ₂ C ₁ Im][OAc]	[Ch][Lys]	[Ch][Lys]
IL purity (wt% of IL in aqueous IL solution	90	10	10
[IL:H ₂ O])			
IL/Biomass ratio (mass ratio on dry basis)	3.6	0.29	0.29
IL recovery (%)	99.9	99.9	99.9
IL price (\$/kg)	5	5	2
Water loading (mass ratio between water and	20	N/A	N/A
biomass in water-wash step in WW route)			
Loss of glucan in water-wash step (wt% of initial	5	NONE	NONE
glucan)			
Loss of xylan in water-wash step (wt% of initial	24	NONE	NONE
xylan)			
Hydrolysis			
Enzyme loading (mg/g glucan present in initial	20	20	10
biomass)			
Enzyme price (\$/kg protein)	4.29	4.29	4.29
Glucan-to-glucose conversion (%)	98	84	90
Xylan-to-xylose conversion (%)	79	80	90
Fermentation			
Co-fermentation of glucose and xylose	YES	NO (only	YES
		Glucose)	
Glucose-to-ethanol conversion (%)	95	90	90
Xylose-to-ethanol conversion (%)	60	0	90

^abased on (Cruz et al. 2013, Li et al. 2013, Li et al. 2015, Shi et al. 2014, Uppugundla et al. 2014)

bconstructed to represent the 'current' one-pot HG process in this study

^cconstructed to represent 'projected' one-pot HG process with perceived advances (esp. with yield and enzyme loading)

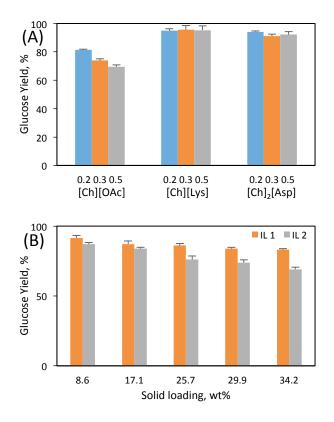


Figure S1. Glucose yields from saccharification of choline-based ionic liquid (IL1: [Ch][Lys]; IL 2: [Ch]₂[Asp]) pretreated corn stover. (A) Glucose yields with different ratios (R: 0.2, 0.3, and 0.5) of biomass to ionic liquid loading in pretreatment; (B) Glucose yield after pretreatment with solid loading from 8.6 to 34.2 wt%.

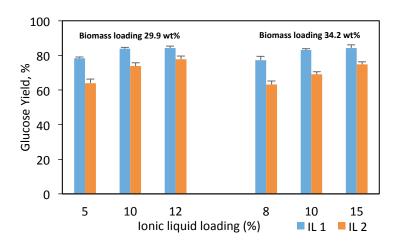


Figure S2. Glucose yields from saccharification of choline-based ionic liquids (IL1: [Ch][Lys]; IL 2: [Ch]₂[Asp]) pretreated corn stover (mass loading of 29.9 wt% and 34.2 wt%) with different ionic liquid loading.

Water-wash route process configuration

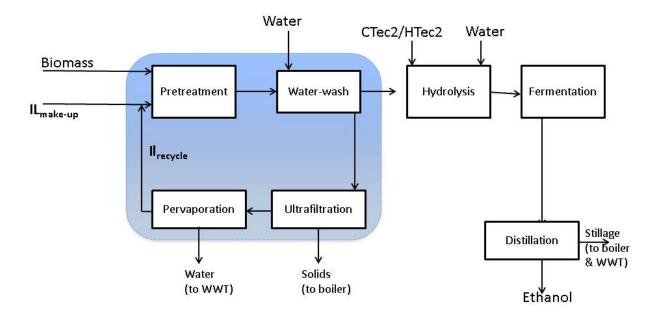


Figure S3. Simplified block flow diagram of water-wash process configuration

One-pot HG process configuration with fed-batch hydrolysis

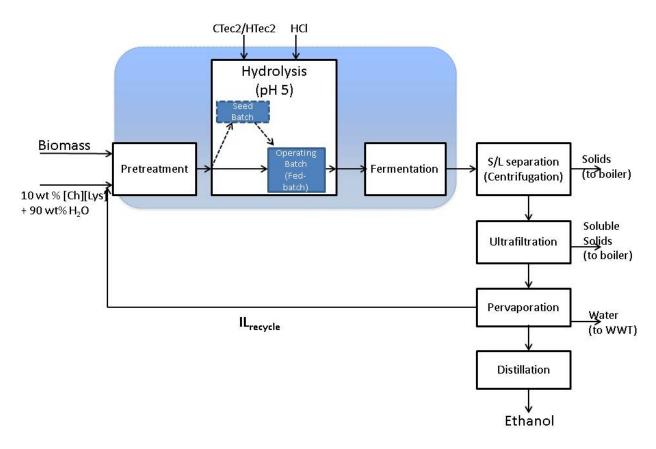


Figure S4. Simplified block flow diagram of one pot HG process configuration

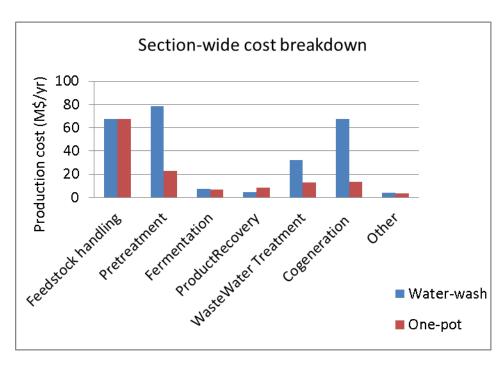


Figure S5. Section wide production costs (including CapEx and OpEx)

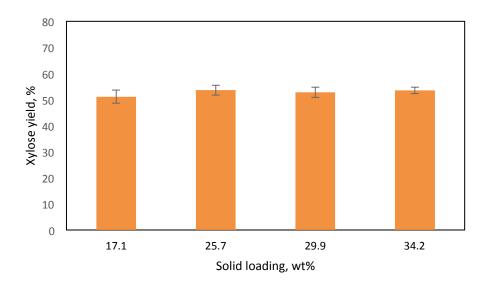


Figure S6. Xylose yields from [Ch][Lys] pretreated corn stover. The ionic liquid loading is 10%.

References

Cruz AG, Scullin C, Mu C, Cheng G, Stavila V, Varanasi P, Xu D, Mentel J, Chuang Y-D, Simmons BA. 2013. Impact of high biomass loading on ionic liquid pretreatment. Biotechnology for biofuels 6: 1-10. Li C, Tanjore D, He W, Wong J, Gardner JL, Sale KL, Simmons BA, Singh S. 2013. Scale-up and evaluation of high solid ionic liquid pretreatment and enzymatic hydrolysis of switchgrass. Biotechnology for biofuels 6: 1-14.

Li C, Tanjore D, He W, Wong J, Gardner JL, Thompson VS, Yancey NA, Sale KL, Simmons BA, Singh S. 2015. Scale-Up of Ionic Liquid-Based Fractionation of Single and Mixed Feedstocks. BioEnergy Research: 1-10.

Shi J, Balamurugan K, Parthasarathi R, Sathitsuksanoh N, Zhang S, Stavila V, Subramanian V, Simmons BA, Singh S. 2014. Understanding the role of water during ionic liquid pretreatment of lignocellulose: cosolvent or anti-solvent? Green Chemistry 16: 3830-3840.

Uppugundla N, da Costa Sousa L, Chundawat SP, Yu X, Simmons B, Singh S, Gao X, Kumar R, Wyman CE, Dale BE. 2014. A comparative study of ethanol production using dilute acid, ionic liquid and AFEX™ pretreated corn stover. Biotechnology for biofuels 7: 72.