## **Supporting Information**

## One-pot pretreatment, saccharification and ethanol fermentation of lignocellulose based on acid-base mixture pretreatment

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**Fig. S1** Effects of the molar ratio of acid–base mixtures using different combinations of acid (HC1, H<sub>2</sub>SO<sub>4</sub>) and base (NaOH, KOH and NH<sub>3</sub>) on the enzymatic digestibility of pretreated and washed rice straw. Pretreatment was performed using various mixing ratios of 0.05 M acid-base mixture at 190°C and a solids loading of 10% (w/v) with 3 min ramping to 190°C and 2 min holding in a microwave digester. Enzymatic hydrolysis was performed using 15 FPU of cellulase (Accellerase 1000) g<sup>-1</sup> glucan at 50°C (pH 4.8) and at 200 rpm for 50 h.







**Fig. S2** Schematic diagrams of various process scenarios. All scenarios and process parameters were on the basis of NREL Technical Report (NREL/TP-5100-47764).<sup>1</sup> Schemes A and B are based on the conventional technologies, which indicate separate conditioning/separate fermentation and separate conditioning/whole slurry fermentation, respectively. Scheme C for whole slurry conditioning and fermentation is the advanced technology that is being tested by NREL.<sup>2,3</sup> Scheme D proposed in the present study is the one-pot pretreatment (using the acid-base mixture), saccharification and fermentation. Estimated costs for each scenario were presented in Fig. 8.



A. SCSF (Separate conditioning and separate fermentation): the conventional scheme

D. ABM one-pot (Acid-base mixture based one-pot): a newly proposed and semi-practical scheme



## Table S1 Estimated costs for the scenarios in Figs. 8 and S2

	SCSF <sup>a</sup>	SCWF <sup>a</sup>	WCF <sup>a</sup>	ABM one-pot <sup>a</sup>
Ethanol price (\$/gal)	6.47	6.42	5.95	5.07
Operating costs (\$/gal)	2.67	2.62	2.15	1.96
Feedstock	0.72	0.76	0.74	0.74
Enzyme	0.36	0.43	0.34 <sup>b</sup>	0.23 <sup>b</sup>
Non-enzyme conversion <sup>c</sup>	1.59	1.43	1.07°	0.99 <sup>c,d</sup>
Installed equipment costs	3.80	3.80	3.80	3.11
Pretreatment	0.49	0.49	0.49	0.55
Neutralization/conditioning	0.05	0.05	0.05	0
Saccharification & fermentation	0.51	0.51	0.51	0
On-site enzyme production	0.30	0.30	0.30	0.34
Distillation and solids recovery	0.37	0.37	0.37	0.41
Wastewater treatment	0.81	0.81	0.81	0.45 <sup>e</sup>
Storage	0.08	0.08	0.08	0.09
Boiler/turbogenerator	1.08	1.08	1.08	1.21
Utilities	0.11	0.11	0.11	0.06 <sup>e</sup>
Ethanol amount (gal/year)	61,000,000	61,000,000	61,000,000	54,591,139 <sup>f</sup>

<sup>a</sup> Values were originated from NREL Technical Report (NREL/TP-5100-47764),<sup>1</sup> and installed equipment costs of SCSF, SCWF and ABM one-pot were based on the cost of WCF.

<sup>b</sup> Enzyme loadings in WCF and ABM one-pot were assumed to be 20 mg/g cellulose and 9 mg/g cellulose, respectively.

<sup>c</sup> Catalysts and neutralizing agents in WCF and ABM one-pot were assumed to be 22.1 mg/g biomass and 4.8 g/L liquor and 16.7 mg/g biomass and 0 g/L liquor, respectively.

<sup>d</sup> The amount of post-wash water usage was assumed to be 30 L/ton biomass<sup>4</sup> and the price of water was assumed to be \$0.4/ton water.<sup>5</sup>

<sup>e</sup> Parameters for time duration was applied (*i.e.* half of total time consuming)

<sup>f</sup>Ethanol production amount was calculated on the basis of the ethanol yield of 70.7% of theoretical maximum.

## References

- 1 D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton and D. Dudgeon, *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover*, National Renewable Energy Laboratory, NREL Technical Report, NREL/TP-5100-47764, Golden, CO, 2011.
- 2 Y. H. Jung, I. J. Kim, H. K. Kim and K. H. Kim, Bioresour. Technol., 2013, 132, 109-114.
- 3 Y. H. Jung, I. J. Kim, H. K. Kim and K. H. Kim, *Bioprocess Biosyst. Eng.*, 2014, 37, 659-665.
- 4 S. Macrelli, J. Mogensen and G. Zacchi, Biotechnol. Biofuels, 2012, 5, 22.
- 5 L. Tao, A. Aden, R. T. Elander, V. R. Pallapolu, Y. Y. Lee, R. J. Garlock, V. Balan, B. E. Dale, Y. Kim, N. S. Mosier, M. R. Ladisch, M. Falls, M. T. Holtzapple, R. Sierra, J. Shi, M. A. Ebrik, T. Redmond, B. Yang, C. E. Wyman, B. Hames, S. Thomas and R. E. Warner, *Bioresour. Technol.*, 2011, **102**, 11105-11114.