Unravelling the Influence of Carbon Dioxide on the Adsorptive Recovery of Butanol from Fermentation Broth using ITQ-29 and ZIF-8

SUPPORTING INFORMATION

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Figure S1. Comparison of experimental values¹ and simulated results for (top) the vapor-liquid equilibrium curve and (bottom) liquid density at 10⁴ kPa of butanol (left) and ethanol (right).



Figure S2: Ethanol adsorption isotherms in DDR zeolite at 303 K (left) and 333 K (right). Comparison of the results obtained with our new model with these obtained experimentally and by simulation in the work of Kuhn *et al.* 2

Table S1: Concentration at the end of fermentation (input values in AspenPlus 4.11) of all components and their mole fraction in the vapor phase (output values) at 35 °C and 5 kPa.

Component	Concentration (g/l)	Mole fraction
	input	output
1-butanol	13.75	1.583 x10 ⁻³
Ethanol	2.56	4.76 x10 ⁻⁴
Acetone	7.04	1.036 x10 ⁻³
butyric acid	0.39	3.74 x10 ⁻⁵
acetic acid	0.38	5.40 x10 ⁻⁵
Water	14.5	0.457109
CO ₂	960.69	0.321173
H ₂	13.75	0.218530



Figure S3: Pore Size Distribution of ITQ-29 and ZIF-8.



Figure S4. Average density profile at (a) 100 kPa and (b) 1000 kPa (total pressure) of ethanol (left) and CO₂ (right) from the CO₂/ethanol binary mixture (99.85:0.15) at 313 K in ITQ-29 (top) and ZIF-8 (bottom). Color gradation indicates occupational density.



Figure S5. Adsorption isotherms from the ternary mixture CO_2 /butanol/ethanol (99.363:0.49:0.147) in ITQ-29 (left) and ZIF-8 (right) at 313 K as a function of total pressure (top) and partial pressure (bottom). Empty symbols correspond to the adsorption isotherms of the CO_2 /butanol (99.5:0.5) binary mixture.



Figure S6. Adsorption isotherms from the ternary mixture CO_2 /butanol/ethanol (99.363:0.49:0.147) in ITQ-29 (left) and ZIF-8 (right) at 313 K s a function of total pressure (top) and partial pressure (bottom). Empty symbols correspond to the adsorption isotherms of the butanol/ethanol (77:23) binary mixture.

REFERENCES

(1) NIST Chemistry WebBook, N. S. R. D. N. E. b. P. J. L., W. G. Mallard 2005.

(2) Kuhn, J.; Castillo-Sanchez, J. M.; Gascon, J.; Calero, S.; Dubbeldam, D.; Vlugt, T. J. H.; Kapteijn, F.; Gross, J. *Journal of Physical Chemistry C* **2009**, *113*, 14290.