

Temperature and Pressure Effects on the Separation Efficiency and Desorption Kinetics in the NH₃-CO₂-H₂O System

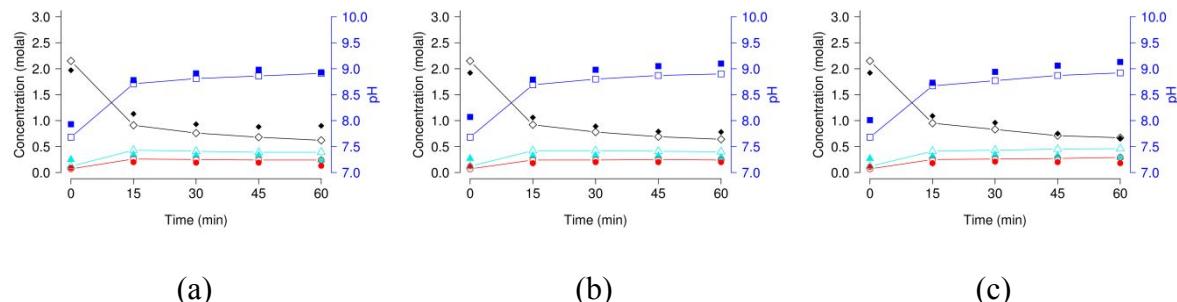
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Supporting Information

The comparison between experimental CO₂ speciation and pH measurements (at 25 °C, 1.01 bar) with the OLI-MSE predicted values (25 °C, 1.01 bar) in NH₃-CO₂-H₂O system for all experimental runs (temperature, pressure) is presented in Figure S1. Table S1 presents the regressed overall desorption rate constants k (min⁻¹) for NH₃ and CO₂ from the NH₃-CO₂-H₂O DDS.



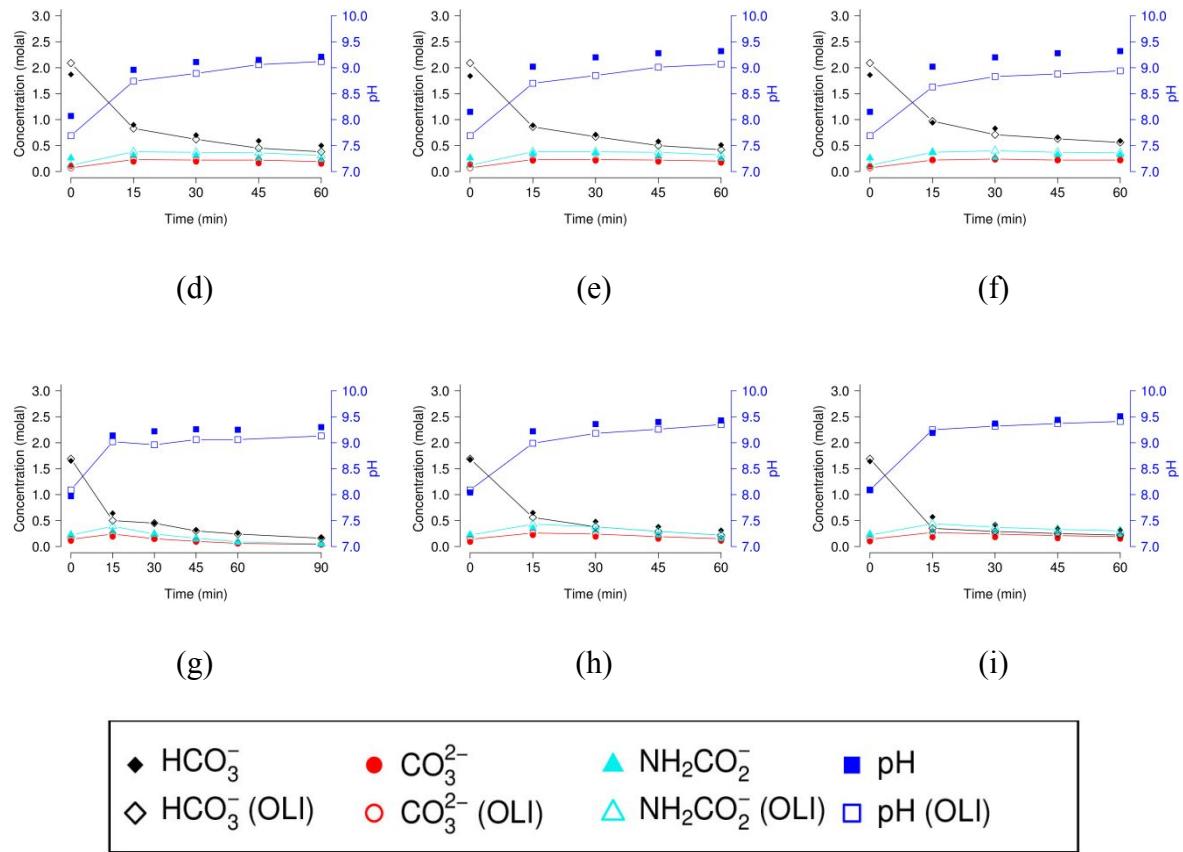


Figure S1 –Experimental CO₂ speciation and pH in NH₃-CO₂-H₂O (measured at 25 °C, 1.01 bar) vs. predicted values (25 °C, 1.01 bar); experimental (temperature, pressure) in (a) (30 °C, 0.35 bar), (b) (30 °C, 0.55 bar), (c) (30 °C, 0.75 bar), (d) (40 °C, 0.35 bar), (e) (40 °C, 0.55 bar), (f) (40 °C, 0.75 bar), (g) (50 °C, 0.35 bar), (h) (50 °C, 0.55 bar), and (i) (50 °C, 0.75 bar)

Table S1 – Overall desorption rate constants k (min^{-1}) for the separation of NH_3 and CO_2 from an
 $\text{NH}_3\text{-CO}_2\text{-H}_2\text{O DDS}$ (15-60 min)

$\text{NH}_3(\text{total dissolved}) \rightleftharpoons \text{NH}_3(\text{g})$ (R18)			
T ($^{\circ}\text{C}$)	P (bar)	k (min^{-1})	R ²
30	0.35	0.0031 ± 0.0005	0.9394
40	0.35	0.0056 ± 0.0004	0.9540
50	0.35	0.0182 ± 0.0003	0.9708
30	0.55	0.0028 ± 0.0003	0.8545
40	0.55	0.0048 ± 0.0006	0.9732
50	0.55	0.0123 ± 0.0010	0.9051
30	0.75	$0.0003 \pm 3.6 \cdot 10^{-7}$	1.0000
40	0.75	0.0042 ± 0.0004	0.8567
50	0.75	0.0063 ± 0.0005	0.9001
$\text{CO}_2(\text{total dissolved}) \rightleftharpoons \text{CO}_2(\text{g})$ (R19)			
T ($^{\circ}\text{C}$)	P (bar)	k (min^{-1})	R ²
30	0.35	0.0054 ± 0.0006	0.9693
40	0.35	0.0105 ± 0.0003	0.9987
50	0.35	0.0198 ± 0.0009	0.9787
30	0.55	0.0047 ± 0.0007	0.9613
40	0.55	0.0100 ± 0.0002	0.9987
50	0.55	0.0168 ± 0.0005	0.9980
30	0.75	0.0041 ± 0.0013	0.8021

40	0.75	0.0068 ± 0.0008	0.9748
50	0.75	0.0090 ± 0.0006	0.9918
