Electronic Supplementary Information for

The Effects of Initial Acetate Concentration on CO₂–Brine–Anorthite Interactions under Geologic CO₂ Sequestration Conditions

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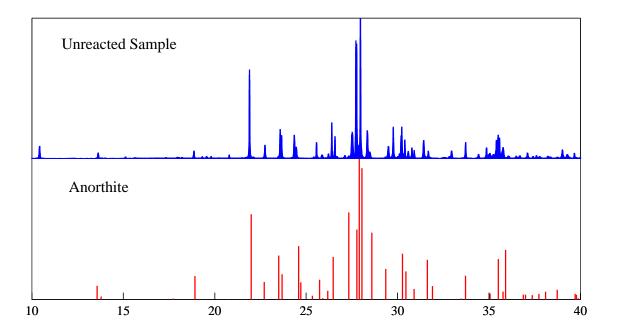


Figure S1. High resolution x-ray diffraction (HR-XRD) pattern of unreacted mineral used in this study. The diffraction pattern for anorthite is shown for reference.¹

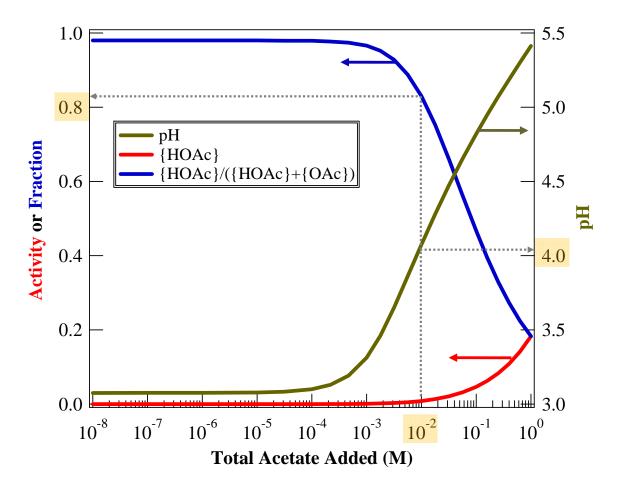


Figure S2. pH buffering effect of acetate added as sodium acetate trihydrate. The speciation diagram is calculated based on thermodynamic data for 35 °C.² The fugacity of CO₂ was estimated according to Allen et al.³ Each corresponding axis for a curve is indicated by an arrow with the same color. The values on the left axis can be used for both the acetic acid fraction (blue line) and the activity of acetate (red line). Given a total amount of acetate added, the pH and the acetic acid speciation of the system can be estimated from the diagram. For example, when 10⁻² M total acetate is added, the pH is ~4.0 (on the black line) and approximately 82% exists as acetic acid (on the blue line). The pH and acetic acid speciation for 0.01 M total acetate added are indicated using grey lines with arrows. The effect of salinity is not accounted for in this diagram.

Table S1. Chemical composition of unreacted mineral used in this study, analyzed by x-ray fluorescence (XRF).

	Wt.%
SiO ₂	51.829
TiO_2	0.121
Al_2O_3	23.673
Fe_2O_3	4.622
MnO	0.086
MgO	3.406
CaO	13.060
Na_2O	3.050
K_2O	0.247
P_2O_5	0.006
Lost in	
Ignition	0.090
(LOI)	0.090
Total	100.182

References

- 1. A. V. Chichagov, *Kristallographiya*, 1990, **35**, 610-616.
- 2. C. M. Bethke and S. Yeakel, *Reference Manual: The Geochemist's Workbench (Release 8.0)*, RockWare, Inc., Golden, 2009.
- 3. D. E. Allen, B. R. Strazisar, Y. Soong and S. W. Hedges, *Fuel Processing Technology*, 2005, **86**, 1569-1580.