### A non-iterative model for H<sub>2</sub>O-CO<sub>2</sub> mutual solubility in chloride brines

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Evaluating the feasibility of  $CO_2$  geologic sequestration requires intensive numerical simulations of multiphase fluid flow. Such simulations involve the calculation of P-T-X data for mixtures of  $CO_2$ ,  $H_2O$  and various salts as a function of temperature, pressure and salinity. A numerically efficient thermodynamic model was developed previously [1] for phase partitioning without salt effects, and was shown to provide an excellent match to experimental data in the range 12–100°C and up to 600 bar. Here, the model is extended to NaCl and CaCl<sub>2</sub> solutions by including activity coefficients for aqueous  $CO_2$  derived from several literature sources. Two of these sources [2,3] yield the best results. The approach allows computing mutual solubilities in a noniterative manner with an accuracy typically within experimental uncertainty for solutions up to 6 molal NaCl and 4 molal CaCl<sub>2</sub> (Figure 1).

Figure 1. Measured (symbols) versus predicted (lines)  $CO_2$  solubilities using five different activity coefficient models.



### References

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# Iodide adsorption and transport at the Hanford Site, Washington

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### Introduction

Because of its long half life  $^{129}\mathrm{I}$  (t<sub>1/2</sub>=1.6x10<sup>-7</sup> years) and high mobility in the subsurface environments, batch adsorption/desorption and flow-through column experiments were conducted for radioactive iodide ( $^{125}\mathrm{I}$  and  $^{129}\mathrm{I}$ ) on sediment from Intergrated Disposal Facility (IDF) which is a proposed low-level radioactive waste disposal facility at the HanfordSite.

### **Results and discussion**

Adsorption experiments conducted with groundwater spiked with dissolved <sup>125</sup>Iodide showed that iodide adsorption was very low ( $K_d$ =0.2 mL/g) at pH 7.5 and decreased with increasing pH. Adsorption linearity was found up to a total concentration of 100 mg/L dissolved iodide. The results of desorption experiments revealed that up to 60 % of adsorbed iodide was readily desorbed from the sediment after 14 days by iodide-free groundwater. The calculated desorption  $K_d$  determined using the ratio of the concentration of iodide in the desorbing solution after 14 days of contact was 1.4 ml/g. The desorption  $K_d$  was significantly greater than the adsorption  $K_d$  of 0.2 ml/g, which indicated that iodide adsorption was not fully reversible at these geochemical conditions (Hanford groundwater at pH 7.5).

Column experiments showed that <sup>129</sup>I transport behavior through the same sediment was slightly retarded compared with that of the non-reactive tracer (<sup>3</sup>H). Slight retardation of <sup>129</sup>I was noticeable in low pore volumes and long tailing was also found in the later stages of the breakthrough curve. The CXTFIT modeling fit to the observed data showed K<sub>d</sub>=0.17 ml/g, consistent with K<sub>d</sub>(0.2 ml/g) obtained from batch experiments.

#### Conclusions

Both batch adsorption and column experiments revealed that  $^{129}I$  was highly mobile at the Hanford Site. The high mobility of  $^{129}I$  is a major consideration in predicting the risks associated with existing and potential future release of  $^{129}I$  to the subsurface geochemical environment at the Hanford Site and other locations.