

# **METAL RELEASE AND TRANSPORT IN POTENTIAL DRINKING WATER AQUIFERS IMPACTED BY STORED CO<sub>2</sub>**

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We present reactive transport simulations of CO<sub>2</sub> leakage from underground storage formations into shallow groundwater aquifers. Dissolution of CO<sub>2</sub> into the groundwater creates carbonic acid and decreases groundwater pH eliciting a geochemical response. Simulations were run using PFLTRAN with different mineral sources of metals (galena and calcite) with multiple realizations of heterogeneous permeability distributions assigned geostatistically to investigate water quality impacts from CO<sub>2</sub> leakage at the basin scale (4 km x 1 km x 0.1 km model domain). Even with fairly coarse grid spacing (~ 9 m x 9 m x 0.9 m), the simulations have > 49 million degrees of freedom and were run on the Jaguar Cray XT5 using 2048 processors.

Simple aquifer mineralogy of quartz with 3% iron oxide and 5% calcite (with 0.1% galena in some cases) was used to isolate sources of pH change and lead to solution. Results from the small ensembles of permeability distribution (5 realizations each of highly stratified and non-stratified aquifers) show that pH decreases more at a pumping well downstream of the leak for aquifers without galena and for highly stratified aquifers relative to non-stratified aquifers. However, in all cases the pH decrease is less than natural variations in pH reported from daily measurements in aquifers. It has been suggested that pH decrease can be used as a diagnostic indicator of a CO<sub>2</sub> leak. However, the studies that provide the basis for this do not account for permeability variations beyond homogeneous layering. Our results suggest that accurate baseline pH is required if pH is to be used as a diagnostic tool for CO<sub>2</sub> leakage. Additionally, pH is a better indicator of CO<sub>2</sub> leakage in highly stratified aquifers than in non-stratified aquifers. Lead concentrations at the pumping well are the same within uncertainty when the source of lead is galena or calcite in highly stratified aquifers. However, in non-stratified aquifers, pumping well lead concentrations are lower when the source of lead is galena compared to trace amounts in calcite. In non-stratified aquifers galena reaches saturation along the flow path before reaching the pumping well and lead concentrations are effectively buffered by low galena solubility. In all of the cases lead concentrations stay well below the maximum contaminant level set by the EPA. Bicarbonate concentrations, another potential indicator of CO<sub>2</sub> leakage, show greater increases in the pumping well when calcite is the lead source relative to when galena is the lead source; likely due to the greater pH decrease in the calcite source simulations. Bicarbonate concentrations nearly double in some cases and in many cases increase by at least 20% suggesting that bicarbonate may be the best geochemical indicator of a CO<sub>2</sub> leak under the conditions simulated here.