

Reactive transport modelling predicting trace metal mobility during CO₂-SO₂-NO-O₂ storage.

KIRSTE, D.¹, PEARCE, J.², DAWSON, G.² AND GOLDING,
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¹ Dept. of Earth Sciences, Simon Fraser University, Burnaby,
BC V5A 1S6, Canada: dkirste@sfu.ca

² School of Earth and Environmental Sciences, University of
Queensland, Brisbane, QLD 4072 Australia:
j.pearce2@uq.edu.au, g.dawson@uq.edu.au,
s.golding1@uq.edu.au

Reactive transport modelling provides an insight into the chemical and physical processes that can take place during the geological storage of CO₂. There is a significant interest in incorporating additional trace gases in the CO₂ stream as well as understanding how those trace gases impact the storage system. In cases where storage systems are linked to groundwater systems that are being utilized for drinking water, there is also a need to determine the potential impacts on water quality in the area of the injected stream and its subsequent migration within the target reservoirs. In this study, reactive transport models were constructed to simulate the injection of CO₂ with SO₂-NO-O₂ coupled with the mobilization and fate of trace elements. Mineral composition, including trace element content and occurrence, was undertaken by conducting bulk chemical characterization, sequential extraction procedures, energy dispersive X-ray spectroscopy, micro-XRF and P-T-X batch experiments. From these, the distribution of trace elements was established, with the majority of the elements of interest (As, Co, Cd, Cu, Mn, Ni, Pb, Zn) occurring in the carbonates, calcite and siderite, in pyrite, and adsorbed on mineral surfaces. Trace elements were incorporated in the models as adsorbed species and as constituents in mineral phases. Thermodynamic data was generated for the mixed composition minerals (carbonates and sulphides) and used in the models to understand the mechanisms of mobilization and transport. The simulations show that significant proportions of the trace elements can be mobilized through carbonate dissolution, consistent with the observations from the batch experiments. Mobility is strongly controlled by adsorption onto surfaces of Fe-oxides and Fe-oxyhydroxides. Within the plume the elements mobilized tend to be rapidly adsorbed resulting in only local changes in the water quality.