

Reactive transport modelling predicting trace metal mobility during CO₂-SO₂-O₂ storage.

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The geological storage of emissions from coal fired power plants could play an important role in reducing the impact of greenhouse gas driven climate change. Prediction of the effects of injection on the physical and chemical conditions in potential storage sites can help inform the risk assessment by identifying possible issues regarding containment and mitigation. Of particular interest is understanding how the target reservoir, the seal and any overlying aquifers may be impacted through gas-water-rock interactions. In this study we focus on the mobilization and fate of trace metals in the reservoir and seal units of the proposed Wandoan pilot site in the Surat Basin, Queensland, Australia. The reservoir and seal rocks and gas-water-rock interactions were characterised through detailed physical and chemical analysis including bulk chemical composition, XRD, QEMSCAN, SEM-EDS and micro-XRF followed by bulk P-T-X experiments. The experiments involved using Parr reactor vessels with variable impurities in the CO₂ stream (+/- SO₂ - +/-O₂). The characterisation allowed identification of the mineral sources of trace metals released during the experiments. Reaction path modelling was conducted to simulate the experiments and thermodynamic and kinetic data were modified to capture the mineral compositions including the trace metal content and the reaction rates. The modified thermodynamic data and kinetic data were used in reactive transport models populated with the physical, hydrogeological and geochemical data of the Wandoan site. The simulations show that the pH is significantly lower proximal to the injector when SO₂ and O₂ are included as impurities when compared to pure CO₂ injection. The low initial SO₂ content (100 ppm) resulted in the majority of SO₂ being partitioned to the aqueous phase closer to the injector. The O₂ transported largely with the CO₂ due to the low solubility and high initial O₂ content (2 %). Chlorite, pyrite and carbonate mineral dissolution resulted in elevated dissolved trace metals content primarily in the reservoir Precipice Sandstone. Precipitation of iron oxides was observed in the experiments and predicted in the simulations. Their role in mitigating trace metals content through adsorption was not yet addressed.

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