Reactive transport modelling of geological storage of CO₂ with impurities: lessons learned

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Abstract

The CO₂ captured from the flue gases of coal fired power plants can contain a range of impurities that may impact the chemical properties and the security of a geological storage system. How the storage system can be affected depends on the solubility and reactivity of the particular impurities. Gases with low solubility and/or reactivity can reduce the CO₂ storage volume by occupying pore space while soluble and/or reactive gases can result in physical (fluid density) and chemical (redox, acidity) changes that could change the storage capacity and security. The most reactive impurities tend to produce strong acids and therefore are considered to be of concern for storage sites as the strong acids will result in increased interaction with the minerals that make up both the reservoir and seal. This can lead to an increased potential for integrity issues around the well bore and the seal as well as pose a risk to groundwater quality if any leakage occurs. Understanding how the impurities might impact a system is critical to ensuring effective and safe storage and one of the most comprehensive approaches used to make an assessment is through reactive transport modelling (RTM). Reactive transport modelling enables predictive evaluation of the impacts but there are significant uncertainties associated with RTM that need to be addressed before confidence in the modelling can be achieved. In this study RTM of injection of CO₂ with SO₂ and CO₂ with NO₂ and O₂ was conducted for a proposed injection and storage site in the Surat Basin in Queensland, Australia. Sensitivity to reactive mineral content, impurity concentration and initial formation water composition as well as mineral reaction rates and reactive surface area was evaluated by generating a series of RTM. Model outputs were found to be particularly sensitive to the reactive mineral content and impurity concentration in the injection stream. The composition of the initial formation water did not have a significant effect except in cases where the alkalinity was very high and resulted in buffering of the acid producing reactions. In the Surat Basin, salinities tend to be relatively low so the range of salinity of the initial formation water was limited and did not affect injectivity through salt formation during dryout. The presence or absence of carbonates was found to be a critical parameter in determining the extent of pH buffering. Even a very small amount of calcite/siderite/ankerite was sufficient to significantly buffer the very low pH induced by presence of impurities in the CO₂ steam and the formation of strong acids. Deciding whether or not a reaction is in equilibrium or controlled by a reaction rate was critical to model output. In particular rates applied to reactions occurring in solution such as redox reactions or gas solution had significant impacts. Without aqueous phase reaction kinetics, differences in the model outputs tended to be predictable where equilibrium controlled reactions resulted in slightly more extensive dissolution/precipitation in the short time scale of the model runs. With aqueous phase reaction kinetics, models conformed better to observations from P-T-X experiments and resulted in more
realistic simulations. Because many of these reactions tend to be proximal to the injector, discretization also played a role in the output. Controlling uncertainty in RTM was critical to increasing confidence in the models. By reducing the uncertainty in the most sensitive components of the models, less sensitive but often more easily constrained aspects could be focussed on and potentially better models would result.