Reactive transport modelling of CO_2 with SO_2 and O_2 as impurities for geological storage: Upscaling from the benchtop to the reservoir

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Carbon capture and storage is proposed to be a means to reduce emissions of CO_2 to the atmosphere. The captured CO_2 stream of coal fired power plants is considered to have impurities at concentrations that range from a few 10's of ppm to a few percent. The presence of impurities can significantly impact not just the physical properties like viscosity and density of the supercritical CO_2 but also the acidity and the redox state of the formation water that the plume comes in contact with. This has very real implications in terms of how the plume migrates and the type and extent of mineral reactions that take place in the reservoir, the seal and in particular, near the well bore. Understanding how these factors will affect the system behaviour is a vital part of the assesment of potential storage sites. Perhaps one of the most useful tools to investigate what could happen is reactive transport modelling (RTM). RTM provides a predictive tool to help understand the chemical and physical behaviour of geologic systems during the storage of CO_2 with impurities. The physical and chemical system presents significant complications that result in very challenging model parameterization that can only be met through careful evaluation of thermodynamic and kinetic data, developing a better understanding of reaction mechanisms and addressing shortfalls in the ability of the RTM codes. Our research is advancing RTM capabilities by conducting experiments investigating how injection of CO_2 with impurities affects reaction pathways and reaction rates, how to upscale through lab experiments to field trials to full scale storage operations and finally, through advancing the numerical modelling codes themselves. Here we summarise the achievements that will ultimately lead to the generation of RTM's of CO_2 injection and storage with impurities like SO_2 and O_2.