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Geochemical reaction path and reactive transport modelling of laboratory experiments in CO_2 storage and mine site monitoring.

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Increasingly, regulators are requiring the development of predictive reactive transport models addressing the potential environmental impacts of resource extraction and waste storage and disposal. The objectives are to assess how these activities pose risks to human and environmental health. The models help not only in the assessment and prediction of those impacts but also in developing strategies for their mitigation. The production of these models requires the physical and chemical characterisation of the materials coupled with static and dynamic experiments to generate an understanding of the processes taking place. Deciding what the appropriate characterisation methods are and the type of experiments best suited to generate an outcome is critical to the production of useful models. In this presentation we will describe the workflow for addressing trace element mobility in the context of CO_2 storage and acid rock drainage that we have found to be useful for reactive transport modelling. Fundamental to the workflow are detailed bulk chemistry, mineralogy, specific mineral composition, and exchange and adsorption site amounts and occupancy analyses. Experiments both static and dynamic are especially useful for determining the type, extent and rate of reactions taking place. Reaction path modelling enables establishing the chemical processes and rates derived from batch experiments while reactive transport modelling of column experiments is vital for establishing the evolution of the fluid composition and the mineralogy that occur through water-rock interactions. The experiments have to be designed so that they mimic the redox state of the system being modelled especially when trace element mobility is an objective of the study. Here we will demonstrate how understanding the minerals and having the appropriate thermodynamic data is critical to producing viable models. Examples from studies on CO_2 storage and acid rock drainage will be used to demonstrate how the process evolves.