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Bridging basic science of geochemical kinetics and applications to CO2 removal and sequestration through geochemical modeling

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Accurate geochemical modeling predictions of CO2 removal from the atmosphere and permanent storage in geological formations via CO2-water-mineral interactions require us to understand both fundamental science of geochemical reactions and modeling tools and databases. On the basic science front, recent innovative research on applying non-traditional stable isotope tracers has broken new ground in near-equilibrium reaction kinetics. Isotope -doping experiments illuminate that irreversible reactions for feldspar weathering reactions mean unidirectional dissolution and how we should model these reactions accordingly [1]. Second, we have recently made a number of geochemical modeling codes and databases are available, which includes SUPCRTBL [2], Online PHREEQC, CO2 Solubility Calculator [3], and H2S Solubility Calculator [4] as well as thermodynamic and kinetic rate constant databases. Notably, the Online PHREEQC program together with our customized databases now allows speciation and solubility and reaction path modeling to temperature up to 1000 oC and pressure up to 5000 bars. This presentation will show these recent studies.

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