Kinetic biogeochemical modeling of a high-pressure reactor simulating H2 geological storages in deep aquifers

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Abstract

If dihydrogen (H_2) is to play a key role in tomorrow's energy mix, massive storage quantities will be required, which can only be achieved by using underground gas storages (UGS), such as deep aquifers.

The main challenge expected with H_2 storage in aquifers is its consumption by microorganisms. Besides consuming the stored energy, these reactions could harm the storage by pressure modification, souring, and modified porosity and permeability via precipitation and dissolution of minerals, as well as bio-clogging. Both recent conceptual modeling and experimental studies underline the need for more experimental data to fit models and upscale them to the aquifer scale.

This work aimed to assess the impact of injecting 2% H_2 over three months into a three-phase high-pressure bioreactor [1,2] simulating the conditions of a deep aquifer with high sulfate concentration (9 mmol/kgw). The built-in capabilities of the PHREEQC software were used to model the liquid-gas and liquid-solid equilibrium, acido-basic, and complexation reactions in a 0D model. New kinetic laws were proposed and implemented into PHREEQC based on microbial taxonomic diversity analyses to model the intricate biotic phenomena observed. This model allows us to represent the growth and decay of the microbial population, respiration rates, and multiple inhibitions.

During this experiment, sulfate reduction occurred until total sulfate consumption, followed by methanogenesis. Formate and acetate production also happened at a slower rate. These reactions consumed 76% of the H_2 quantity injected. However, while H_2 remained in sufficient quantity, the microbial activity stopped after the total consumption of all electron acceptors and alkalinization (pH 9.5). We hypothesize competition for CO_2/carbonates between microorganisms and geochemical processes (i.e., mineral precipitation). This suggested that H_2 could be stable in this aquifer after an initial loss. Although sulfate reduction induced notable sulfide production, all the sulfide produced was attenuated, probably through the precipitation of pyrite. The developed model represents a preliminary step toward a comprehensive description of H_2 fate in the underground, allowing for an upscaled reservoir model in a second step.

[1] Haddad et al. 2022, Energy Environ. Sci. 15, 3400.

[2] Mura et al. 2024, International Journal of Hydrogen Energy. 63, 330.