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The effect of pH on the kinetics of D/H isotopic exchange between molecular hydrogen and water

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Molecular hydrogen (H_2) is now being considered as a carbon-free fuel and energy vector with the potential to play a key role in the energy transition. In the Earth's subsurface, natural H_2 emissions, dominantly produced from water-rock reactions, have been observed in a variety of geological settings. The measured isotopic composition of (white) H_2, given as D/H ratio or D, varies from ~-995‰ to ~-50‰ [1]. This wide range is influenced by a variety of processes, including kinetic isotope effects associated with H_2 formation, destruction, and equilibration with water, the latter proceeding at fast (order year) timescales at low temperatures (<100°C). It is generally assumed that in geologic settings, H_2 is found in isotopic equilibrium with local waters such that the D of H_2 (i.e., D_{H2}) is set by D of local waters (i.e., $D_{H2O(l)}$) and temperature of the system. This temperature dependent distribution, termed the fractionation factor ($^{D}_{H2O(l)\text{-}H2(g)}$), is commonly used as a geothermometer for subsurface H_2 formation or re-equilibration temperatures.

Here we will present new experimental data on the kinetics of D-H exchange for H_2 dissolved in liquid water at temperatures below 100°C along with our recently published calibration of hydrogen isotope equilibrium between H_2 and liquid water [2]. Specifically, we are conducting experiments in a flexible gold reaction cell (i.e., Dickson-type apparatus) at low temperature (<100°C) under neutral and alkaline pH conditions (pH = 7 and 10) to test the role of OH^- in setting the speed of exchange. These systems do not have a headspace and allow for continuous sampling. We will compare our new results with previous experiments and discuss the effect of pH on the kinetics of D/H isotope exchange and its implication for subsurface hydrogen generation, in particular from low temperature serpentinization which is the most likely source of H_2 in alkaline springs.

1. Gibson, J. J., et al., (2024). *International Journal of Hydrogen Energy*, *66*, 468-478.
2. Hochscheid F., et al., (2025). *Geochimica et Cosmochimica Acta.* In press.