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A microcontinuum reactive transport model for understanding H_2 production during serpentinization on Earth and Mars

CORALIE VESIN AND BENJAMIN M. TUTOLO
University of Calgary

Serpentinization of ultramafic bodies occurs worldwide on Earth, and has been observed on other planetary bodies in the Solar System, including Mars. This reaction is of particular interest for the associated H_2 production, which is regarded as a potential source of energy for the future, and also thought to have played a role in the creation of habitable environments and, potentially, the emergence of life. The H_2 is a by-product of the oxidation of ferrous iron, initially in olivine and orthopyroxene, to ferric iron in magnetite and serpentine.

As demonstrated by many experimental studies, the chemical and physical properties of the serpentinization system, including the protolith composition, element activities, fluid salinity, porosity, temperature, and pH, influence the reaction characteristics. For instance, Fe-rich protolith are prone to generate more H_2 during serpentinization, and is enhanced at elevated temperatures, pH, and fluid salinities. It has also been frequently observed that, while Mg-rich terrestrial peridotites are typically completely serpentinized, Fe-rich serpentinites are only partially serpentinized, impacting the extent of the H_2 production.

A comprehensive understanding of the Fe partitioning during serpentinization and the drivers of the complete reaction are essential to elucidate the mechanisms of H_2 production. These intricate interactions and reactive feedback call for a better comprehension of the serpentinization on the microscale, at each step of the reaction. In this study, we develop a reactive transport model in coherent and consistent geochemical systems representing terrestrial peridotite (Mg-rich) and Martian crust (Fe-rich) compositions. A tailored thermodynamic database is used, compiled with the PyGeochemCalc package and encompassing the mineral phases, solid-solutions, gases, and aqueous species of interest, at 0−350°C and 350 bars. Representative samples of terrestrial serpentinized peridotites and Mars analogue samples are investigated with imaging-based techniques including scanning electron microscopy and Raman spectroscopy. This approach facilitates the quantification of the microporosity and the volume fractions and reactive surface areas of the minerals. Along with the chemical properties, the geometry of the system can then be implemented in the reactive transport model performed with PFLOTRAN.