Characterization of elemental release during interaction of bacteria with basalt and granite

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We used batch reactors to characterize the rates and mechanisms of elemental release during the interaction of a single bacterial species (*Burkholderia fungorum*) with basalt and granite at T = 28°C for 36 days. We supplied glucose as a C source, either NH_4^+ or NO_3^- as N sources, and trace apatite in the rocks as a P source. We measured the release of Al, Ca, F, Na, Mg, P, Si, and Sr under several biotic and abiotic conditions with the aim of evaluating how actively metabolizing bacteria might influence basalt and granite weathering on the continents. Over the entire experimental period, reactors containing viable bacteria yielded the highest elemental release rates. Large pH decreases occurred when using NH_4^+. No pH changes occurred when using NO_3^-. We attribute pH lowering to either organic acid production or H^+ extrusion during NH_4^+ uptake. Protons may be produced and consumed simultaneously during NO_3^- uptake, resulting in a net zero pH change. Elemental release rates inversely correlate with pH, suggesting that proton-promoted dissolution was the dominant reaction mechanism. In the granite reactors, formation of Al-F and Fe-F complexes may have enhanced mineral solubility by lowering Al and F activities. Within the context of this study, bacteria appear to elevate the rate of long-term atmospheric CO_2 consumption by Ca-Mg silicate weathering between factors of 2 and 5 over corresponding inorganic rates. The effect is greater for basalt than granite. With respect to the granite experiments, we propose that microbially enhanced Ca release from apatite and fluorite may contribute to elevated Ca/Na ratios commonly observed in granitic watersheds.

Ab initio molecular dynamics study of Li speciation in aqueous fluid at high pressure

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Fluids play an important role in almost all geochemical processes, such as dissolution and precipitation of minerals, isotopic fractionation or mass transport in hydrothermal systems. A key parameter for a quantitative understanding of fluid properties and geochemical processes involving aqueous fluids is the complexation of the dissolved ions and molecules. Since the speciation does not only depend on the chemical composition, but also on pressure and temperature, any direct approach for studying the molecular structure and transport in fluids at conditions of the Earth's interior requires in situ experimental techniques (e.g. x-ray diffraction, x-ray absorption, Raman and infrared spectroscopy). However, most of these methods are insensitive to low concentrations of light elements, such as Li. Recently, due to the massively increased computing power, ab initio molecular dynamics (AIMD) simulations have become a powerful technique for molecular modeling of fluids with a complex chemistry that are nor well described by classical models.

Here, the hydration of a Li ion in aqueous fluid is studied as a function of pressure by AIMD simulation at constant temperature (T=1000 K) and constant volume. The pressure is derived from an equation of state of pure H_2O fluid. The calculations show that structural changes of the H_2O fluid in the studied pressure range from P=3 kbar to P=60 kbar also affect the hydration of the Li ion. Since the number of H_2O molecules in the first hydration shell of the Li ion is subject to rapid dynamic change, a distribution of coordination numbers can be calculated for each pressure. With increasing pressure, the average coordination number increases with considerable decrease of 3- and 4-fold and respective increase of 5- and 6-fold coordinated Li. The ionic coordination changes in aqueous fluids as a function of pressure could affect the isotopic fractionation between minerals and fluids and consequently could have implications for models of the geochemical element cycles. As a test of the possible P-dependence of the Li-isotope fractionation, experimental studies on the model system spodumene - fluid are currently being performed and will be discussed.