Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.37375

A first principle thermodynamic framework to describe organic ligand promoted dissolution of aluminosilicates

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A method for decreasing CO_2 in air and water is mineralisation as carbonate phases. A promising approach is geologic carbon capture and immobilisation in basaltic rocks, such as CarbFix (www.carbfix.com). Enhanced weathering projects have gained increasing attraction in the past decade. The success of these approaches relies inherently on answering the following questions: How much CO_2 can be captured and how can these processes be accelerated? A key step in mineralisation is the dissolution of aluminosilicate materials and subsequent release of divalent cations, which react with dissolved CO_2 to form carbonates. Currently, dissolution models are mostly empirical and therefore constrained to the conditions in which they were developed. A gap between laboratory and field derived rate laws remains, which is partly a result of the complexity of conditions found in nature, one of which is the presence of organic ligands. A more fundamental understanding of organic ligand promoted dissolution could help close this gap.

An alternative to empirical fitting of experimental rates is the use of a microkinetic model. Instead of using empirical parameters to fit experimental dissolution rates, one can use first principle modelling to derive thermodynamic parameters that can predict rates over a broad range of conditions. We used density functional theory (DFT) to investigate the effect of organic ligand-surface complexation and implemented it in an existing microkinetic model [1], creating a general thermodynamic framework to describe ligand enhanced dissolution. We validated the approach by comparing our results with experimental dissolution rates of basaltic glass in the presence of citrate/citric acid for different concentrations over a pH ranging from 2 to 12 (Figure 1). The work contributed insight into the effects of organic ligands where the functional groups are carboxyl and hydroxyl. Future work will investigate molecules with other functional groups. The overall goal is to learn what defines an effective organic catalyst for silicate dissolution, to hasten and optimise CO_2 mineralisation.

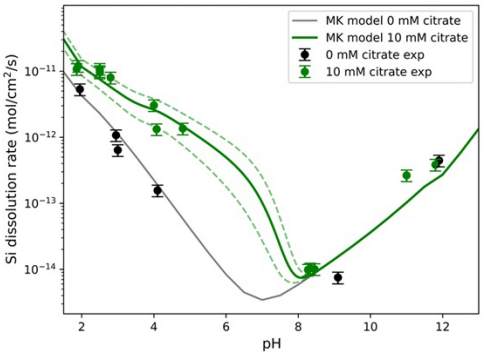

Figure 1: Modelled basaltic glass dissolution rate with and without the presence of citrate.

References

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