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Learning the factors controlling mineral dissolution in three-dimensional fracture networks

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We perform a set of high-fidelity simulations of geochemical reactions within three-dimensional discrete fracture networks (DFN) and use various machine learning techniques to determine the primary factors controlling mineral dissolution. The DFN are partially filled with quartz that gradually dissolves until quasi-steady state conditions are reached. At this point, we measure the quartz remaining in each fracture within the domain as our primary quantity of interest. We observe that a primary sub-network of fractures exists, where the quartz has been fully dissolved out. This reduction in resistance to flow leads to increased flow channelization and reduced solute travel times. However, depending on the DFN topology and the rate of dissolution, we observe substantial variability in the volume of quartz remaining within fractures outside of the primary subnetwork. This variability indicates an interplay between the fracture network structure and geochemical reactions. We characterize the features controlling these processes by developing a machine learning framework to extract their relevant impact. Specifically, we use a combination of high-fidelity simulations with a graph-based approach to study geochemical reactive transport in a complex fracture network to determine the key features that control dissolution. We consider topological, geometric and hydrological features of the fracture network to predict the remaining quartz in quasi-steady state. We found that the dissolution reaction rate constant of quartz and the distance to the primary sub-network in the fracture network are the two most important features controlling the amount of quartz remaining. This study is a first step towards characterizing the parameters that control carbon mineralization using an approach with integrates computational physics and machine learning.

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References

Primary author: Dr PACHALIEVA, Aleksandra (Los Alamos National Laboratory)

Co-authors: O'MALLEY, Daniel; Dr SRINIVASAN, Gowri (Los Alamos National Laboratory); VISWANATHAN, Hari (Los Alamos National Laboratory); HYMAN, Jeffrey (Los Alamos National Laboratory)

Presenter: Dr PACHALIEVA, Aleksandra (Los Alamos National Laboratory)

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