Specifying rate constants and reaction path on the water-rock chemical reaction based on exchange Monte Carlo method and sparse modeling

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Water-rock interaction in surface and subsurface environments occurs in complex multicomponent systems and involves several reactions, including element transfer. Such kinetic information is obtained by fitting a forward model into the temporal evolution of solution chemistry or the spatial pattern recorded in the rock samples, although geochemical and petrological data are essentially sparse and noisy. Therefore, the optimization of kinetic parameters sometimes fails to converge toward the global minimum due to being trapped in a local minimum.

In this study, we present a novel framework to estimate multiple reaction-rate constants from the mineral distribution pattern in a rock by using the exchange Monte Carlo method (Hukushima & Nemoto, 1997; Iba, 2001). We applied the method to the synthetic data, which includes nine unknown parameters to be estimated (Oyanagi et al., 2018). As a result, probabilistic distribution of six unknown parameters among them showed normal distributions and the proposed method could find each true parameter. However, the probabilistic distribution of others showed uniform distributions and the proposed method failed to estimate each true value because these parameters did not contribute to the observed dataset. We suggest that effective reaction paths could be extracted from mineral distribution pattern in a rock, by excluding non-effective rate constant using a sparse Modeling.

References

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