Approximate Bayesian Computation of surface-area model selection in water-rock interactions

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Water-rock interaction is one of the key ingredients in understanding the dynamic processes of surface and subsurface environments of the Earth. It has been, however, frequently remarked that there exist several orders of discrepancy in kinetic rates between laboratory and fields, which is attributed to a large uncertainty in estimates of the surface areas in the various geological situations.
In order resolve the problem, it is highly desired to establish an analytical method which provides an accurate estimation of the kinetic rate constant from reaction solvent data obtained by laboratory and also fields. In particular, it is of significant for the considered method to have an ability to identify a model of the surface areas.
In this study, we firstly applied Approximate Bayesian computation (ABC) method to select model of surface areas of minerals and evaluate the reaction rate constant from the solution chemistry data. ABC has recently attract attention in the field of machine learning as an efficient inference technique for some problems in which a likelihood function is difficult to evaluate. Here, we discuss one of the simplest chemical reaction systems which is realized in laboratory experiments. Chemical equations are given by a set of ordinary differential equations for each chemical constituent concentrations. For a given set of reaction rate constants and an initial condition, time evolution of the concentrations is obtained relatively easily in numerical simulations, while to evaluate the likelihood function under an observation noise is a non-trivial task. This is the situation that ABC should work effectively. We propose a framework to evaluate the reaction rate constants from partially observed data for the case where time evolution of an intermediate product is only observable from experimental measurements. Actual numerical calculations are based on a population-type Monte Carlo method which is one of various technique in the ABC scheme. It is found that the proposed method successfully evaluates the rate constants for a synthesis data of the intermediate product. In addition, we show some results of the model selection of the surface areas on the basis of ABC.

Keywords: water-rock interactions, Approximate Bayesian Computation, surface-area model

