SCG62-02 Room:502 Time:May 2 09:15-09:30

Numerical modeling of water-rock reaction with a focus on the earth's surface environment

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Water-rock interaction proceeds by the interplay between dissolution/precipitation, diffusion of ions, and water flow in rock pores. The reaction-transport process in rock is quantitatively described by:

$$\phi(\partial c/\partial t)= D_e(\partial^2 c/\partial x^2)-v\phi(\partial c/\partial x)+Ar_0 f(c)$$

This equation is an example of the one-dimensional reaction-transport equation, and c is the solute concentration (mol/cm^3), t is the time (s), x is the distance (cm), ϕ is the porosity (dimensionless), D_e is the effective diffusion coefficient (cm^2/s), v is the flow rate in pores (cm/s), A is the surface area per unit volume of rock (cm^2/cm^3), r_0 is the rate constant (mol/cm^2/s). $f(c)$ is the function that expresses the concentration dependence of the dissolution rate (mol/cm^2/s), and for quartz, $f(c)=(1-c/c_{eq})$ (c/c_{eq} is the equilibrium Si concentration) (Scott et al., 2009). By solving the reaction-transport equation, we can know how the distributions of the solute concentration and dissolution rate and the amounts of primary and secondary minerals change with time. Such analysis is called the reactive transport modeling and has been applied to the studies of various processes including soil formation (Maher et al., 2009) and the reactions associated with geologic storage of CO_2 (Xu et al., 2010).

The parameters used in the reaction-transport equation can be estimated by direct measurement in the field, laboratory experiment, and fitting in the modeling. To reproduce natural process accurately, we need to estimate each parameter as precisely as possible. However, it is difficult to evaluate what value is most proper. For example, the reactive surface area A is often determined by measuring the volume of gas adsorbed on the mineral or by approximating the geometry of the mineral. However, the proportion at which the reactive surface area determined by these processes contributes to actual reaction is often unclear. In addition, there are cases where various $f(c)$ have been proposed for a specific mineral and the dissolution rate varies with time (White and Brantely, 2003). In such case it is unclear what equation should be used. Therefore, the way of setting appropriate parameter is one of the main subjects of research.

In water-rock reaction on the earth's surface environment, evaluation of the effect of water saturation is important because water saturation changes dynamically as a result of the occurrence of intermittent drying and infiltration. It has been reported that both the hydraulic conductivity and effective diffusion coefficient in rock decrease with decreasing water saturation and this significantly affects the result of the reactive transport modeling (Yokoyama, 2013). In addition, how water saturation affects the reactive surface area has been revealed recently (Nishiyama and Yokoyama, 2013).

Keywords: Reactive transport modeling, Water-rock reaction