

Mathematical modeling of reactive transport in porous media with mineral precipitation-dissolution

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The description of reactive transport problems in porous media on the field scale requires models consisting of partial differential equations, describing e.g. advection, diffusion and reactions of chemical species. These equations have to represent processes taking place on the pore and on the molecular scale. When reactions with minerals are involved, some specific challenges arise with respect to the mathematical model and its numerical solution:

First, for minerals, considered as constant activity species, it has to be distinguished between the two cases of a mineral being present, which allows for dissolution, and the mineral being completely dissolved, which prohibits any further dissolution. In a mathematical model these two cases can be formulated in an elegant way by a so-called complementarity condition. Such a formulation is useful for implementation of a numerical code, but also for mathematical analysis of the model. Complementarity formulations are useful both for a kinetic description and for an equilibrium formulation of the mineral reaction. Second, often the assumption is made that the reaction rate depends on the size of the reactive surface, which again is related to the mineral volume. Measurements may lead to assumptions such as $A(m) \sim m^\alpha$ with $0 < \alpha < 1$, where m is the mineral volume or mass and $A(m)$ is the surface area. Geometric arguments, e.g., assuming a hemispherical shape of the nuclei, may lead to $A(m) \sim m^{2/3}$. However, relations of this shape lead to models with non-unique solutions, i.e., to ill-posed problems, and numerical results are not reliable. We show how to avoid this severe issue, i.e., it is possible to reformulate the model in a well-posed form, providing uniqueness, and also non-negativity of the solution. Finally, we will discuss models which go beyond the simple assumption that the surface is a function of the mass. Such models have to describe the microscopic process of precipitation-dissolution in more detail, e.g., by introducing a model for nucleation and by considering a population of nuclei and keeping track of the individual grain sizes. It seems that such a model does not suffer from non-uniqueness issues.