Abstract

Several real-world problems originating from the fields of chemical engineering, material sciences, soil mechanics, reservoir flow, groundwater flow, etc. can be studied in the context of porous media flow. In this thesis, we start with a pore-scale model where two mobile species with different diffusion coefficients react and precipitate as an immobile species (crystal) on the grain boundary. The reverse process of dissolution is also happening and we consider a multi-valued dissolution rate term to describe the dissolution process. The modeling of such transport processes leads to a coupled system of parabolic partial differential equations together with nonlinear multivalued ordinary differential equations. We first proved the global existence of the weak solution for this system and upscaled the system from the microscale to the macroscale so that we can compute numerical simulations efficiently. The process of going from micro to macro scale description is called homogenization. We derived several corrector results to justify the homogenization process. Furthermore, we performed numerical simulations to compare the outcome of the effective model with the original heterogeneous microscale model. We then generalized the system by considering space and time-dependent different diffusion coefficients. We have shown the global existence of weak solutions with the help of Rothe's method and we also did the homogenization of the system by applying rigorous upscaling techniques such as two-scale convergence and periodic unfolding.

Towards the end of this thesis, we established the global existence of the non-negative classical solutions of a highly nonlinear reaction-diffusion system. We addressed the case for $I(>2)$ number of dissolved chemical species and $J(>1)$ number of chemical reactions happening among them. We considered measurable and uniformly bounded nonidentical diffusion coefficients and the system of reversible reactions with non-homogeneous Neumann boundary conditions. The system is assumed to satisfy only the mass control condition and to have locally Lipschitz nonlinearities with arbitrary growth. The main novelty of this work is that we did not assume the closeness of the diffusion coefficients. We utilize the regularization of the heat operator and the duality method to derive the result. We also illustrate the global in-time bounds for the solutions.

Keywords: reactive transport, diffusion-reaction-dissolution-precipitation, global weak solution, periodic homogenization, corrector estimates, numerical simulation, two-scale convergence, boundary unfolding operator, classical solution, mass control