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Numerical investigation of a fully coupled two-scale model for mineral dissolution and precipitation

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Mineral dissolution and precipitation alter a porous medium's structure and its bulk properties. Due to the medium's heterogeneity and lacks in dynamic pore-scale measurements, there has been an increasing interest in comprehensive models accessing such phenomena on the macroscale without disregarding available pore-scale (micro-scale) information. Such micro-macro models may be derived from detailed pore-scale models applying upscaling techniques and comprise several levels of couplings. Our model consists of transport equations for dissolved chemical species at the scale of the porous medium (macro scale) while taking the processes of convection and diffusion into account. They include averaged time- and space-dependent coefficient functions such as porosity and the effective, potentially anisotropic diffusion tensor. These coefficient functions are in turn explicitly computed by means of auxiliary cell problems (micro scale). Structural changes due to mineral dissolution and precipitation reactions result in a time- and space dependent domain on which cell problems are defined. We characterize the interface between the mineral and the fluid and consequently the explicit geometric structure by means of a level-set. Its evolution depends on the transport equations' solutions, i.e. the chemical species' concentrations (micro-macro scale).

A numerical scheme is introduced which enables evaluating such complex micro-macro settings. For the level-set equation an upwind scheme by Rouy and Tourin is applied. An eXtended Finite Element Method is used for the evaluation of the cell problems while the transport equations are solved applying Mixed Finite Elements. Ultimately, we investigate the potentially degenerating bulk properties of the medium such as porosity and effective diffusion. Moreover, we apply our approach to the dissolution of an array of calcite grains in the micro-macro context and validate our numerical scheme.