NUMERICAL INVESTIGATION OF A FULLY COUPLED MICRO-MACRO MODEL FOR MINERAL DISSOLUTION AND PRECIPITATION

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We investigate multiscale models describing mineral dissolution and precipitation processes. Such multiscale models may be derived from detailed pore-scale models applying upscaling techniques. Since mineral reactions alter the porous medium's structure and its bulk properties, the models comprise several levels of couplings. Our model consists of transport equations at the scale of the porous medium (macroscale) while taking the processes of convection, diffusion and reaction into account. They include averaged time- and space-dependent coefficient functions which are in turn explicitly computed by means of auxiliary cell problems (microscale). Structural changes due to dissolution and precipitation reactions result in a time- and space-dependent domain, on which cell problems are defined. The interface between the mineral and the fluid, and consequently the explicit geometric structure, is characterized by means of a level set. Here, information from the transport equations' solutions is taken into account (micro-macroscale). A numerical scheme has been developed which enables evaluating such complex settings. Within this framework the potentially degenerating bulk properties of the medium such as porosity, diffusivity and permeability could be investigated. To reduce computational costs, adaptive methods for controlling the macroscopic steps are investigated. Moreover, we applied our approach to the dissolution of an array of calcite grains in the micro-macro context and validated our numerical scheme.

References

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