Numerical Upscaling of Reactive Transport with Applications to Geochemistry

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Introduction

Reactive flows in porous media are an important process in many industrial and environmental applications. The reactive transport in porous media is influenced by the interplay between convection, diffusion and reaction, coupled with the heterogeneity of the pore space and chemical heterogeneity. Understanding these processes at different scales, and how they interact, poses a number of research challenges. In this talk, we will discuss the upscaling of reactive transport in complex domains, which often arise in geological applications.

First, we will present the software PoreChem, which is used for the simulations and calculations and discuss the workflow needed for using it in practical upscaling scenarios. Second, we will give an overview over the topic of homogenization of reactive transport, especially using the method of asymptotic expansion. Then, we will show recent results on pores-scale simulation of reactive transport in complex domains and the solution of the relevant cell problems for homogenizing passive and reactive transport. Finally, we will show an example with an application to reactive transport of MCPA in a soil sample and we will give computational results and discuss comparisons to experiments.

Pore-Scale Simulation

To perform the simulations Fraunhofer ITWM has developed PoreChem [1,2], a software package dedicated to the simulation of reactive flow on the pore-scale. It enables the simulation of reactive flows in resolved porous media in a reasonable time. The software can compute the flow of a fluid in the pore space, as well as the diffusive and advective transport of a solute species. Reactions can then be simulated occurring not only in the fluid volume but also on the surface of the porous medium and on interfaces between two fluid phase regions. The flow is computed by solving the Navier-Stokes-Brinkman system of equations with a finite volume discretization on a regular voxel grid. Transport and reactions are simulated by solving the reaction-diffusion-advection equation with the same discretization coupled to the surface concentration by Robin boundary conditions. For the reactions, different reaction kinetics, parametrized by reaction isotherms can be taken into account. The fast voxel based solver enables calculations directly on µCT-Images.

Numerical Upscaling of Reactive Transport

The upscaling of reactive transport has been studied for a long time and is a well-established field. Various mathematical techniques have been developed, among the most prominent of which are volume averaging, the method of moments and upscaling by asymptotic expansion. In this talk, we will shortly review application of the asymptotic expansion method to transport problems (see e.g. [3,4]), and show how different scaling regimes lead to different cell-problems [5], which have to be solved to compute effective diffusion and dispersion tensors. Then we show how, using PoreChem, the relevant cell problems can be solved numerically and effective diffusion and dispersion tensors can be computed.

Results

As a geophysical application, we consider adsorption of 2-methyl-4-chlorophenoxyacetic acid (MCPA) in Geothite. The starting point for the study are a 3D µCT-Image of a soil sample, containing reactive and non-reactive surfaces. Detailed chemical computations are made using the software PHREEQC. Then, a simplified Henry Isotherm model is fitted to the results, which is the used to compute reactive flow on the µCT-Images. Computational studies (see Figure 1) are carried out for different pH-Values, and local results are shown together break through curves. Then, upscaling of the problem is discussed by defining the relevant cell problems and showing their solution (see Figure 2). A comparison with experimental data is also discussed. Finally, we give an outlook on outstanding problems and possible extensions of the models.

References

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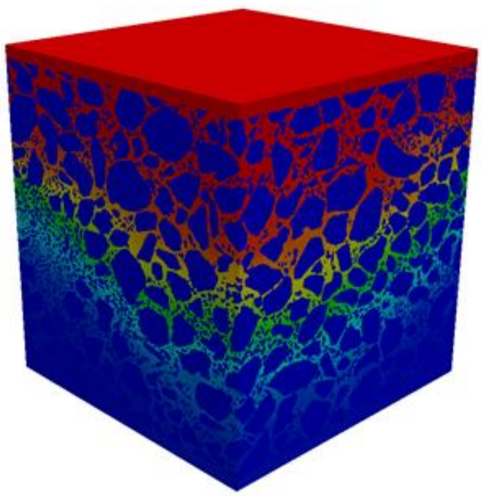

Figure 1: Pore-Scale simulation of reactive transport of MCPA in a soil sample.

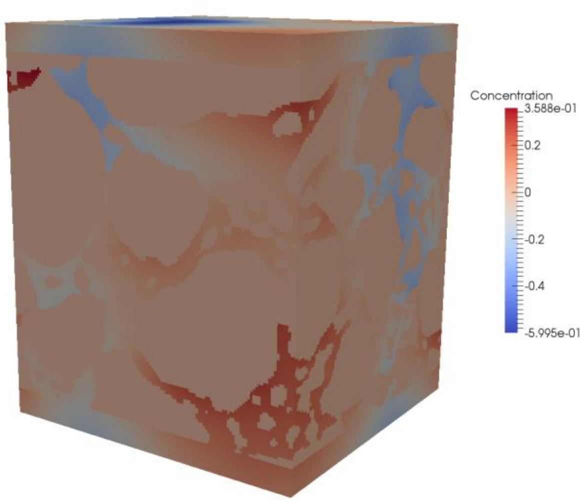

Figure 2: Solution to a diffusion/dispersion cell problem in a soils sample.