Multiscale dynamics of reactive fronts in the subsurface

FINAL REPORT

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1. Brief summary of progress to date.

Major Goals of the Project. Overreaching goals of the proposed activity are to develop an or- ganizing framework to describe nonlinear reactive transport in geologic systems over many length and time scales, and corresponding physics-based adaptive multi-scale hybrid models. We will also provide computational tools for robust uncertainty quantification in hybrid simulations.

Major Activities of the Project. The major activities in this reporting period have focused on developing a time-averaging framework for ADR transport (Task 1) and global diagnosis criteria for spatio-temporal algorithm refinement (Task 2), as well as numerical validation and verification of the analytical approaches developed. The main activities are as follows:

(a) We use homogenization theory to perform a spatio-temporal upscaling of pore-scale advection- diffusion equation in a periodic porous medium in the presence of fluctuating boundary conditions on some parts of the boundary and nonlinear chemical reaction on the solid-liquid interface and we investigate the constraints under which the macroscopic equation gives an accurate explanation of the underlying physics at the pore scale. We demonstrate that the dynamics at the continuum scale is strongly influenced by the interplay between signal frequency at the boundary and transport processes at the pore level. Furthermore, we show that by choosing appropriate scaling factors, a homogenized equation along with expressions for the effective coefficients reliably describe the concentration of solute at the length and time scales vastly different from physically robust micro-scale provided that some specific scale separation constraints are met. Our analysis proves that if the reaction rate or advection at the micro-scale are large, the effectiveness of the homogenized model is impeded.

(b) We test numerically the conditions derived theoretically for advective-diffusive and reactive trans- port in a fracture with planar walls subject to temporally oscillating Dirichlet boundary conditions. The numerical analysis confirms the theoretical predictions.

Significant Results. Two paper are in preparation.

2. Description of work yet to be accomplished

The Tasks yet to be accomplished are listed below:

(a) Quantify the impact of uncertainty in wall geometry of planar fractures on predictions hybrids of ARD transport

(b) Develop coupling conditions for time hybridzation

(c) Quantify the impact of uncertainty in pore geometry on predictions of hybrids of ARD transport in porous media, i.e. develop stochastic hybrid models

(d) Use the hybrids combined with X-Ray tomographic images of pore scale structure (from Dr. Gouze, see letter of collaboration) to model dynamic changes in porosity/permeability