# A NOVEL COMPUTATIONAL FRAMEWORK FOR BIMOLECULAR DIFFUSIVE-REACTIVE SYSTEMS

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Mixing of chemical species across plume boundaries has a major influence on the fate of the reactive pollutant in the subsurface flow. Small-scale heterogeneity and anisotropy lead to irregular plume boundaries, which enhances mixing-controlled reactions through increasing the interfacial area of the plume. Therefore, it is crucial to capture heterogeneity and anisotropy in order to properly model reactive transport in hydrogeology. One can resolve heterogeneity through mesh refinement or by employing multiscale methods (e.g., Arbogast (2000), Chen and Hou (2003), Aarnes (2004)). In this talk, we shall concentrate on the numerical challenges due to anisotropy in predicting the fate of chemical species.

We will present a novel non-negative computational framework for diffusive-reactive systems in anisotropic rigid porous media. The governing equations for the concentration of reactants and product will be written in terms of tensorial diffusion-reaction equations. We shall restrict our talk to fast irreversible bimolecular reactions. We employ a linear transformation to rewrite the governing equations in terms of invariants, which are unaffected by the reaction. This results in two uncoupled tensorial diffusion equations in terms of these invariants, which are solved using a novel non-negative solver for tensorial diffusion-type equations. The concentrations of the reactants and product are then calculated from invariants using algebraic manipulations. Several representative numerical examples will be presented to illustrate the robustness, convergence, and the performance of the proposed computational framework. We will also compare the proposed formulation with other popular formulations. In particular, we will show that the standard single-field formulation does not produce reliable solutions, and the reason can be attributed to the fact that the single-field formulation does not guarantee non-negative solutions. We will also show that the clipping procedure (which produces non-negative solutions but is considered as a variational crime) over predicts the plume length.