Geophysical Research Abstracts
Vol. 15, EGU2013-5652, 2013
EGU General Assembly 2013

Pore scale simulation and upscaling of reactive transport in disordered porous media

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Formal upscaling from pore to continuum scale of the basic equations governing reactive transport requires invoking several assumptions. Length and time scale separation is required to allow considering average quantities as representative of pore scale distributions. Likewise, the magnitude of the Damköhler and Péclet numbers should satisfy some requirements. If these conditions are not met, the advection dispersion reaction equation (ADRE) cannot be used in its standard formulation and some alternative models should be employed. Here, we focus on a simple reactive transport problem involving a homogeneous bimolecular irreversible reaction of the kind $A+B\rightarrow C$. This problem involves a very simple chemical reaction pattern, but provides a useful benchmark against which one can test the accuracy of continuum scale reactive transport models which are usually implemented at the large scale. The process is simulated at the pore scale in two-dimensional disaggregated porous media constituted by ordered and disordered arrays of cylinders. A particle tracking approach is employed to model transport subject to advection, molecular diffusion and homogeneous reactions between chemical species. Pore scale results are then used to verify the appropriateness of continuum scale models, which can be derived from volume averaging of the key pore scale equations. The appropriate format of continuum scale models depends on specific combinations of Damköhler and Péclet numbers. This is evidenced by the observation that (a) the reactive process may influence the (effective) dispersive transport coefficients, and (b) incomplete mixing of the reactants at the pore scale needs to be included in the upscaled reaction term in the presence of fast reactions. These issues are discussed via a detailed analysis of our pore scale simulations results. An assessment of the influence of the pore scale geometry configuration on the system parameters is provided. We compare results obtained by simulating the process in two-dimensional porous media of increasing complexity. We focus on the analysis of the process development in disordered media, which are characterized by the alternation of stagnant regions and channels where advective effects are relevant. These configurations enable us to identify the effect of the heterogeneous distribution of the pore scale velocity field on the dynamics of the reactive process. Our results allow assessing the appropriateness of the investigated continuum scale formulations and may provide a guidance in quantifying the effect of pore scale heterogeneities on the associated effective model parameters.