Characterization of bimolecular reactive transport in heterogeneous porous media

YANIV EDERY[1], GIOVANNI M. PORTA[2], ALBERTO GUADAGNINI[2], HARVEY SCHER[1], BRIAN BERKOWITZ[1]*

1. Department of Earth and Planetary Sciences, Weizmann Institute of Science, 7610001, Rehovot, Israel
2. Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano, Milano, Italy

(*correspondence: brian.berkowitz@weizmann.ac.il)

We characterize the role of preferential pathways in controlling the dynamics of bimolecular reactive transport in a representative model of a heterogeneous porous medium. We examine a suite of numerical simulations that quantifies the irreversible bimolecular reaction $A + B \rightarrow C$, in a two-dimensional heterogeneous domain (with log-conductivity, Y), wherein solute A is injected along an inlet boundary to displace the resident solute B under uniform (in the mean) flow conditions. Preferential pathways most distinctly emerge with increasing degree of heterogeneity of the system (as expressed by the unconditional variance, σ^2_Y) and act as channels to focus the encounter and reactions between A and B particles. We explore the feedback between the reactive process and (a) the degree of system heterogeneity, as quantified by the unconditional variance of Y, $1 \leq \sigma^2_Y \leq 7$, representing moderately to strongly heterogeneous media; and (b) the relative strengths of advective and diffusive mechanisms, as quantified by a grid Péclet number, Pe_Δ. Our analysis is based on identification of particle preferential pathways, focusing on particle residence time within cells employed to discretize the flow domain. These preferential pathways are formed mainly by high conductivity cells, and generally contain an important component of (sometimes isolated and a relatively small number of) lower conductivity values. While the former dominate the behavior, the latter are shown to provide a non-negligible contribution to the global number of reactions taking place in the domain for strongly heterogeneous media, i.e., for the largest investigated values of σ^2_Y. Low conductivity zones in the preferential pathways contribute to trapping B particles and delaying their encounter with A particles, which takes place when B particles enter adjacent cells residing within the preferential pathways by slow advection or diffusion. Reactions are detected across the complete simulation time window (of about 5.5 pore volumes) for the strongly advective case. When diffusion plays an important role, the reactive process essentially stops after the injection of a limited amount (~2.5) of pore volumes.