Models – Repositories of Knowledge
(Proceedings ModelCARE2011 held at Leipzig, Germany, in September 2011) (IAHS Publ. 355, 2012), 163-168.

Compound-specific local and effective transverse dispersion coefficients for conservative and reactive mixing in heterogeneous porous media

GABRIELE CHIOGNA[1,2], OLAF A. CIRPKA[2], PETER GRATHWOHL[2] & MASSIMO ROLLE[2]

1 University of Trento,Dipartimento di Ingegneria Civile ed Ambientale, via Mesiano 77, I-38123 Trento, Italy
gabriele.chiogna@ing.unitn.it

2 University of Tübingen,Center for Applied Geosciences, Sigwartstr. 10, D-72076 Tübingen, Germany

Abstract Dilution in heterogeneous porous media can be quantified using different measures which lead to the definition of effective dispersion coefficients. These up-scaled parameters should account for both local-scale dispersion and effects of flow variability in heterogeneous formations (e.g. flow focusing in high- conductivity and defocusing in low-conductivity inclusions). The correct quantification of mixing is particularly important in order to model mixing-controlled reactions in porous media. Under steady-state conditions with continuous injection from a line source, 2D conservative and reactive solute transport simulations were performed. It was shown that different parameterizations of local transverse dispersion coefficients significantly affect the quantification of field-scale mixing processes. Bench-scale experiments showed a nonlinear dependence of local transverse dispersion on molecular diffusion over a wide range of flow velocities, implying compound-specific transverse mixing at the local Darcy scale. Heterogeneous field-scale scenarios were considered, characterized by different variability in the conductivity field, and a set of Monte Carlo simulations was performed. We quantified transverse mixing with different measures including effective transverse dispersion coefficients, scalar dissipation rates and the recently introduced flux-related dilution index and flux-related second central spatial moments. It was shown that quantities derived in a flux-related framework are affected by a lower degree of uncertainty and that, in the case of low to moderately heterogeneous porous media, the effective transverse dispersion coefficients are significantly different for different compounds. Effective transverse dispersion coefficients were found to be up to one order of magnitude larger than the local values due to mixing enhancement processes related to flow-focusing in high-permeability inclusions. In the case of mixing-controlled reactive transport, considering instantaneous complete bimolecular reactions, it was shown that compound-specific dispersion coefficients affect the prediction of the length of reactive solute plumes. Furthermore, the recently developed concept of critical dilution index was applied to quantify the amount of mixing required to completely degrade a reactive contaminant plume.

Key words mixing; transverse dispersion; dilution index