Upscaling diffusion effects in groundwater transport: An investigation from pore to field scale

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Mixing processes significantly affect and limit conservative and biogeochemical reactive transport of contaminants in the subsurface. The goal of this study is to investigate the role of diffusion and compound-specific mixing for solute transport in groundwater at different scales, including: (i) pore-scale (~ 10^{-2} m), (ii) laboratory bench-scale (~ 10^{0} m) and (iii) field-scale (~ 10^{2} m). We investigate both conservative and mixing-controlled reactive transport using pore-scale modeling, flow-through laboratory experiments and field-scale numerical modeling in complex heterogeneous hydraulic conductivity fields. We consider different steady-state and transient transport scenarios. For the conservative cases we use, as metric of mixing, the exponential of the Shannon entropy to quantify solute dilution either in a given volume (dilution index) or in a given solute flux (flux-related dilution index). The mass and the mass-flux of a reaction product as well as the extent of reactive plumes are evaluated to quantify reactive mixing. The results show that diffusive processes occur at the small-scale of a pore channel but also manifest at larger macroscopic scales. The outcomes of our study illustrate the need to consider and properly account for compound-specific diffusion and mixing limitations in order to accurately describe and predict conservative and reactive transport in porous media.