Mixing, dispersion and reaction under transient flow conditions

Marco Dentz[1], Maria Pool[1], and Vincent Post[2]
[1]Institute of Environmental Assessment and Water Research, Spanish National Research Council, Barcelona, Spain
[2]BGR - Federal Institute for Geosciences and Natural Resources, Hanover, Germany

ABSTRACT

Mixing and dispersion in coastal aquifers are strongly influenced by temporal flow fluctuations on time scales ranging from daily (tides), seasonal (pumping and recharge) to glacial cycles (regression and transgressions). Temporal flow fluctuations under medium compressibility and spatial heterogeneity lead to a complex space and time-dependent flow response which induces enhanced mixing and dispersion of dissolved substances. We analyze effective mixing and solute transport in temporally fluctuating flow for a stable stratification of two fluids of different density using detailed numerical simulations and column experiments. The dispersion and mixing behaviors are quantified in terms of the evolution of the interface width, the mixing rate (rate by which concentration variance is destroyed), and the distribution of concentration point values. Furthermore, we consider the efficiency of the dissolution of calcite under high Damköhler numbers, this means under mixing-limited conditions. For spatially homogeneous aquifers, we find that mixing and dispersion are mainly controlled by the hydraulic diffusivity, the period of the transient forcing, and the initial interface location. At short times, mixing can be characterized by a constant effective dispersion coefficient and both the interface position and width evolve linearly in time. For increasing times, we observe sublinear increase of the interface width, which indicates interfacial compression. This behavior is caused by a deceleration of the interface as it intrudes into the aquifers. This deceleration is caused by the fact that the flow velocity decreases exponentially with distance from the flow boundary as a consequence of compressibility of the porous matrix. We quantify the observed mixing behaviors and interface evolution by a time-averaged model that is obtained from a two-scale expansion of the full transport problem, and derive explicit expressions for the center of mass and width of the mixing zone between the two fluids [Pool et al., 2016]. For spatially heterogeneous media, we observe that the global mixing and reactivity are on the order of or even smaller than for homogeneous media, which can be traced back to heterogeneity-induced fluid segregation [Pool et al., 2018]. At the same time, we observe a strong local enhancement of the mixing and reaction rates, which increases with the connectivity of the hydraulic conductivity field. The tendency to extreme mixing and reaction rates is manifested in the distribution of point of values of the spatially distributed mixing and reaction rates. The local maxima of the mixing and reaction rates are localized in regions of strong interface deformation, which correspond to high velocity zones and therefore also large dispersion. Density variations lead to an additional interface compression, which in turn emphasizes local maxima in mixing and reaction rates. Our results provide quantitative evidence that the deformation of the interface induced by spatial heterogeneity and transient flow fluctuations coupled with density variations leads to the formation of complex patterns of reaction hotspots, zones of enhanced reaction efficiency, whose distribution is linked to the medium structure and the deformation properties and topology of the flow field. Our work provides new insights into the role of spatial and temporal variability on the mixing and reaction efficiency as well as the formation of geochemical reaction patterns in heterogeneous environmental systems.

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Contact Information: Marco Dentz, Institute of Environmental Assessment and Water Research (IDAEA), Spanish National Research Council, c/ Jordi Girona 18, 08034 Barcelona, Spain. Email: marco.dentz@csic.es, website: https://mhetscale.wordpress.com