Geophysical Research Abstracts
Vol. 18, EGU2016-1026, 2016
EGU General Assembly 2016

Effects of incomplete mixing on chemical reactions under flow heterogeneities.

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December 1, 2015

Abstract

Evaluation of the mixing process in aquifers is of primary importance when assessing attenuation of pollutants. In aquifers different hydraulic and chemical properties can increase mixing and spreading of the transported species. Mixing processes control biogeochemical transformations such as precipitation/dissolution reactions or degradation reactions that are fast compared to mass transfer processes. Reactions are local phenomena that fluctuate at the pore scale, but predictions are often made at much larger scales. However, aquifer heterogeities are found at all scales and generates flow heterogeneities which creates complex concentration distributions that enhances mixing.

In order to assess the impact of spatial flow heterogeneities at pore scale we study concentration profiles, gradients and reaction rates using a random walk particle tracking (RWPT) method and kernel density estimators to reconstruct concentrations and gradients in two setups. First, we focus on a irreversible bimolecular reaction $A + B \to C$ under homogeneous flow to distinguish phenomena of incomplete mixing of reactants from finite-size sampling effects. Second, we analise a fast reversible bimolecular chemical reaction $A + B \rightleftharpoons C$ in a laminar Poiseuille flow reactor to determine the difference between local and global reaction rates caused by the incomplete mixing under flow heterogeneities.

Simulation results for the first setup differ from the analytical solution of the continuum scale advection-dispersion-reaction equation studied by Gramling et al. (2002), which results in an overstimation quantity of reaction product (C). In the second setup, results show that actual reaction rates are bigger than the obtained from artificially mixing the system by averaging the concentration vertically.

- LITERATURE

Gramling, C. M.,Harvey, C. F., Meigs, and L. C., (2002). Reactive transport in porous media: A comparison of model prediction with laboratory visualization, Environ. Sci. Technol., 36, 2508?2514.