Geophysical Research Abstracts
Vol. 18, EGU2016-1019, 2016
EGU General Assembly 2016

Modelling transport in media with heterogeneous advection properties and mass transfer with a Continuous Time Random Walk approach

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Transport processes in groundwater systems are strongly affected by the presence of heterogeneity.
The heterogeneity leads to non-Fickian features, that manifest themselves in the heavy-tailed breakthrough curves, as well as in the non-linear growth of the mean squared displacement and in the non-Gaussian plumes of solute particles. The causes of non-Fickian transport can be the heterogeneity in the flow fields and the processes of mass exchange between mobile and immobile phases, such as sorption/desorption reactions and diffusive mass transfer. Here, we present a Continuous Time Random Walk (CTRW) model that describes the transport of solutes in d-dimensional systems by taking into account both heterogeneous advection and mobile-immobile mass transfer. In order to account for these processes in the CTRW, the heterogeneities are mapped onto a distribution of transition times, which can be decomposed into advective transition times and trapping times, the latter being treated as a compound Poisson process.
While advective transition times are related to the Eulerian flow velocities and, thus, to the conductivity distribution, trapping times depend on the sorption/desorption time scale, in case of reactive problems, or on the distribution of diffusion times in the immobile zones. Since the trapping time scale is typically much larger than the advective time scale, we observe the existence of two temporal regimes. The pre-asymptotic regime is defined by a characteristic time scale at which the properties of transport are fully determined by the heterogeneity of the advective field. On the other hand, in the asymptotic regime both the heterogeneity and the mass exchange processes play a role in conditioning the behaviour of transport.
We consider different scenarios to discuss the relative importance of the advective heterogeneity and the mass transfer for the occurrence of non-Fickian transport. For each case we calculate analytically the scalings of the breakthrough curves and of the moments of the particles displacements in both the pre-asymptotic and the asymptotic regimes and we study the spatial distribution of particles. Analytical results are compared with numerical particle tracking simulations.