Geophysical Research Abstracts
Vol. 21, EGU2019-5570-1, 2019
EGU General Assembly 2019

Stochastic dynamics and upscaling of anomalous dispersion in heterogeneous porous media from the Darcy to the regional scale

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The prediction of large scale solute dispersion in porous media is a key issue for a series of environmental and industrial applications ranging from groundwater management to geological storage and energy production. This understanding is complicated due to spatial heterogeneity in hydraulic conductivity, which may span up to 12 orders of magnitude. Using a stochastic modeling approach for the medium heterogeneity, we extract the salient features of the random motion of solute particles through a systematic statistical analysis of particle velocity series measured equidistantly along streamlines. The velocity series form an ergodic and stationary Markov process, which can be parameterized by a characteristic velocity length scale and the Eulerian velocity distribution, this means in terms of medium and flow properties. This finding renders the streamwise particle motion a time-domain or continuous time random walk type process because particles move across a constant spatial increment during random times, which are determined by the Markovian random velocity. We investigate the impact of medium heterogeneity and the initial solute distribution on the preasymptotic and asymptotic transport in terms of breakthrough curves, the spatial solute distribution and the evolution of its streamwise mean and variance. We compare the data of direct numerical flow and transport simulations to the stochastic particle model in order to evaluate its predictive capabilities. Based on the stochastic particle model, we present explicit (semi-) analytical results for the scaling of the breakthough curves as well as expressions for preasymptotic and asymptotic dispersion behaviors for weakly and strongly heterogeneous conductivity fields. The stochastic particle dynamics can be cast into a deterministic Boltzmann-type equation for the average solute concentration. The presented approach sheds some new light on the mechanisms of solute dispersion in heterogeneous porous media. Furthermore, it provides an efficient predictive upscaled model for large scale solute dispersion in highly heterogeneous media that can be conditioned on the heterogeneity in the injection domain.