The Effect of Velocity Correlation and Marginal Velocity Distribution on Transport in Heterogeneous Media: A Copula-Based Approach

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Introduction

In heterogeneous media, the velocity distribution and the spatial correlation structure of velocity for solute particles determine solute breakthrough curves and how they may evolve as one moves away from the solute source. Thus, the ability to model this evolution can help relating the statistical hydraulic properties of the media to the transport behavior and travel time distributions. While commonly used non-local transport models such as anomalous dispersion and classical continuous time random walk (CTRW) approaches reproduce breakthrough curves successfully they are often not able to account for the evolution of breakthrough curves as a function of distance. This in turns limits the transferability of these models. In the research to be presented, we express concentration or flux of solutes as a distribution over their velocity. We then derive an integro-differential equation that governs the evolution of the particle distribution over velocity at given times and locations for a particle ensemble, based on a presumed velocity correlation structure and an ergodic cross-sectional velocity distribution. This way, the spatial evolution of breakthrough curves away from the source is predicted based on cross-sectional velocity distribution and the connectivity, which is expressed by the velocity transition probability density. The transition probability is specified via a copula function that can help construct a joint distribution with a given correlation and given marginal velocities. Using this approach, we analyze the breakthrough curves depending on the velocity distribution and correlation properties. The model shows how the solute transport behavior evolves from ballistic transport at small spatial scales to Fickian dispersion at large length scales.

Theory

The methodology presented is based on deriving a governing equation for the evolution of concentration distribution over velocity based on a Lagrangian expression of velocity transition. It can be shown that if we express the velocity evolution over a streamline in a Lagrangian framework as:

\[ v(s + \Delta s) = \zeta(s)v(s) + [1 - \zeta(s)]\nu[v(s)] \]

where \( \zeta(s) \) is a Bernoulli random variable that takes the values 1 with probability \( p_r = \exp(-\Delta s/\epsilon) \) and 0 with probability \( 1 - p_r \); \( \epsilon \) is a persistence length and the velocities \( \nu(v) \) are positive random variables that are conditioned on the velocity \( v \) according to \( \nu(v) \propto p_v(v | v) \), then the upscaled transport equation for \( c(v) \) expressing the concentration distribution over velocity \( v \) can be written as:

\[
\frac{\partial c(v; x, t)}{\partial t} + v \frac{\partial c(v; x, t)}{\partial x} = D \frac{\partial^2 c(v; x, t)}{\partial x^2} + \frac{v}{\epsilon} \int dv' p(v | v') c(v'; x, t) - \frac{v}{\epsilon} c(v; x, t)
\]

where \( D \) is the molecular diffusion coefficient. Note that the integral of the concentration over velocity (i.e. \( \int c(v)dv \)) is the flux weighted concentration at a given cross-section at a given time. We can now express the cumulative joint distribution of the velocity before and after a transition event using a Copula function as:

\[
P(v, v') = \Upsilon[P(v), P(v')]
\]

where \( \Upsilon \) is a copula function which is monotonic with respect to both its arguments and is defined over the domain \([0, 1] \times (0, 1] \rightarrow [0, 1] \) and \( P_v \) is the cumulative marginal velocity distribution. Using the chain rule the non-cumulative joint distribution of velocity before and after a transition can be written as:

\[
p(v, v') = p_v(v)p_v(v')\phi[P_v(v), P_v(v')]
\]

where \( p_v \) is the marginal velocity density and \( \phi \) is the copula density function (i.e the derivative of \( \Upsilon \) with respect to both its arguments. Substituting Eq. (4) into Eq. (2) yields:

\[
\frac{\partial c(v; x, t)}{\partial t} + v \frac{\partial c(v; x, t)}{\partial x} = D \frac{\partial^2 c(v; x, t)}{\partial x^2} + \frac{v}{\epsilon} \int dv' p_v(v)\phi[P_v(v), P_v(v')]|v' = x, t - \frac{v}{\epsilon} c(v; x, t)
\]
Now imposing a variable transformation \( u = P_v(v) \) Eq. (5) can be written in terms of the corresponding value to the cumulative marginal velocity distribution as:

\[
\frac{\partial c(u; x, t)}{\partial t} + v(u) \frac{\partial c(u; x, t)}{\partial x} = D \frac{\partial^2 c(u; x, t)}{\partial x^2} + \frac{\partial v(u)}{\partial x} \int_0^1 du' \phi(u, u') c(u'; x, t) - \frac{v(u)}{\epsilon} c(u; x, t)
\]  

(6)

where \( c(u) \) and \( c(v) \) are related via:

\[
c(u) = p_v(v) c(v)
\]  

(7)

and the flux-weighed concentration can be found by taking the integral of \( c(u) \) from 0 to 1.

1 Results

Figure 1 shows normalized breakthrough curves obtained at various distances from the source based on a spike release where the velocity correlation is considered to be expressed via a Gaussian copula with a correlation factor of 0.36. Panels (1) and (c) are based on a power-law marginal velocity distribution with an \( \alpha \) parameter of 2.5 and panels (b) and (d) are based on a log-normally distributed marginal velocity distribution.

![Figure 1: Normalized breakthrough curves obtained using particle tracking based on Gaussian copula with a correlation length scale \( l_c \) equal to the transition length scale \( \epsilon \) (i.e Gaussian copula correlation parameter \( r = 0.36 \)) based on (a) and (c) truncated power-law distribution and (b) and (d) Lognormal distribution with a shape factor \( \sigma \) = 0.5. \( \tilde{v} \) is the median marginal velocity.]

References