Identification of transition-rate probability distributions for transport from macroscopic experimental observations

Andrea Cortis

September 5, 2006

Contaminant transport in geological formations can be effectively described by means of the time convolution of the classical advection-dispersion equation with a time-memory function $M(t)$. In the Continuous Time Random Walk (CTRW) formalism, $M(t)$ is intimately related to $\psi(t)$, the probability distribution function of the contaminant transition rates. The $\psi(t)$ maps the structure of the unresolved spatial heterogeneities into a distribution of transition rates. Direct observation of the $\psi(t)$ at the pore scale represents a formidable experimental challenge. First principles theoretical derivations of the $\psi(t)$ represent a daunting task and only a few explicit solutions exist. Simple analytical models for the $\psi(t)$ depending on a small number of parameters have been therefore postulated, based on asymptotic transport considerations. The model parameters can be easiliy identified by means of least squares optimization of the CTRW solutions on experimental data (e.g., breakthrough curves, concentration profiles).

Hydrogeological systems such as fracture networks in permeable rocks, karst systems at high Reynolds numbers, and channeling in Darcy flow (to mention only a few), however, cannot be treated by means of these simple $\psi(t)$ models.

In this work, we present a novel methodology for the identification of the full spectrum of the $\psi(t)$ from macroscopic experimental observations. This deconvolution technique provides a new and powerful tool for the investigation of the influence of heterogeneous structures on the macroscopic transport parameters.

This work was supported by the U.S. Department of Energy under contract No. DE-AC03-76SF00098.