A Direct Time-Domain Particle Tracking Method for Modeling Solute Transport in a Network of Fractures

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Modeling of solute transport in naturally fractured rocks is challenged by a suitable description of the inherent heterogeneity and associated uncertainty of the fracture network. Despite the success of discrete fracture network (DFN) models in reproducing geometric and structural properties of a fracture network, the extensive computational load of DFNs on numerical simulation of solute transport inevitably limits themselves to small-scale applications. Therefore, we have developed a direct time-domain particle tracking (TDPT) method for overcoming these difficulties. Transport processes considered in our TDPT model includes advection and hydrodynamic dispersion in the fracture and Fickian diffusion in the matrix. Mass exchange between fracture and matrix is also assumed by molecular diffusion. Decay and kinetic sorption onto fracture surfaces and within matrix pores are considered as well. This approach is different from other TDPTs in that particle arrival time can be sampled directly by a single step, and that hydrodynamic dispersion is taken into account for a reliable prediction of particle travel time. The 'directedness' of our TDPT is achieved by neglecting aperture variability within a single fracture and by incorporating hydrodynamic dispersion into the transport model. Note, however, that a heterogeneous aperture field within the network is allowed in order to reflect large-scale flow channeling caused by velocity variation between fracture segments. We also derive a memory function to represent the retention process due to kinetic sorption and Fickian diffusion into rock matrix of limited size. Laplace domain transport model is first solved from a Lagragian perspective, which is then numerically inverted to get the particle arrival time. Simulation results in a single fracture show that early-time BTC characteristics are determined mainly by transport in the fracture. On the other hand, late-time BTC is controlled by retention-related processes such as sorption and matrix diffusion into and out of rock matrix of limited size. For a single fracture with a larger penetration depth, particles need a longer time to saturate the matrix and then diffuse back to the fracture. Accordingly, on a log-log plot, the late-time BTC shows an obvious slope change that virtually results in a flat curve with finite width. This phenomena is clearly different from tracer transport in fractured rocks with infinite rock matrix. Preliminary sensitivity analysis indicates that the significance of retention depends on matrix porosity, molecular diffusion coefficient, distribution coefficient in matrix, and fracture aperture. These parameters can be lumped to a dimensional parameter similar to the diffusion parameter used in the single fissure dispersion model (SFDM) for solute transport in a single fracture with infinite rock matrix. The power of the above direct approach is its fast speed of computation. For example, on a PC with a single-core CPU, only less than 0.02s is needed to complete calculations for 10,000 particles across a single fracture. Besides single fracture simulations, this method is also applied to a simple hypothetical 2D fracture network. Results show that, in addition to penetration depth, geometric properties of a single fracture and network connectivity are two factors that significantly affect BTC characteristics no matter in travel time variance, peak concentration, peak arrival time, and BTC tailing.