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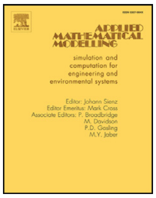

Coarse-scale particle tracking approaches for contaminant transport in fractured rock

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ABSTRACT

Random-walk particle tracking methods are frequently used for modeling contaminant transport, as relevant to radionuclide transport in fractured rock. Standard particle-tracking methods need to be modified for handling discontinuities in velocity and diffusion coefficients as at fracture–matrix interfaces, and handling these discontinuities accurately requires time steps much smaller than the diffusion time scale across narrow fracture apertures. In this work we present coarse-scale particle tracking methods that exploit the contrast in diffusivities between fracture and rock matrix to allow the use of time steps much larger than the diffusion time scale across fracture apertures. Thus, they reduce computational effort by several orders of magnitude. We develop two coarse-scale versions of the standard particle tracking method, one applicable to particles starting in the fracture, and another to particles starting in the rock matrix. The two methods can be used in combination to track particles through individual fractures, including the influence of matrix diffusion. The main advantage of our methods result from the computationally efficient treatment of (two-way) fracture–matrix particle transfer. These methods can also be combined with existing particle tracking approaches for complex advection–diffusion–dispersion in fractures to handle fracture–matrix interactions efficiently.

1. Introduction

Contaminant transport in fractured rock masses is relevant in the context of protecting groundwater resources and safety assessments of nuclear waste repositories, several of which are being sited in subsurface geologic media [1]. Modeling contaminant transport in fractured rock is hampered by difficulties in constraining the precise geometry of fracture networks, flow/transport properties of individual fractures, and fracture–matrix diffusive exchange. Approaches to modeling contaminant transport in fractured rock include equivalent porous-medium, dual or multi-continuum and discrete fracture network (DFN) models [2]. Of these approaches, the DFN models are the most computationally demanding since they represent the underlying fracture network at high resolution. While they represent fundamental transport processes at highest resolution, their drawback is that DFNs cannot be characterized precisely in field settings, and statistical representations are required. Characterizing the risk associated with contaminant transport will thus require simulations on several realizations of fracture networks (the same is true of the other classes of models as well).

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Nomenclature

pdf	probability density function
χ	indicator function
C_f	contaminant concentration within fracture
C_m	contaminant concentration within matrix
a	fracture half-aperture
D	free molecular diffusion coefficient
D_e	effective diffusivity in rock matrix
ϕ	porosity of rock matrix
$\bar{u}$	velocity within fracture averaged over fracture width
t	time coordinate
T	non-dimensionalized time
x	spatial coordinate aligned with the fracture
y	spatial coordinate perpendicular to the fracture
s	distance perpendicular to fracture wall
Δt	time step size
Δt_m	portion of time step spent within matrix
Δt_f	portion of time step spent within fracture
Δt_{FPT}	time step calculated from a first passage time distribution
r_N	random variable $\sim \mathcal{N}(0,1)$
r_u	random variable $\sim \mathcal{U}(0,1)$

With the advent of modern high-performance computing, large-scale simulations on multiple realizations of discrete fracture networks is becoming increasingly feasible, even with millions computational nodes to resolve channeling within individual fractures [3] and representation of fracture–matrix interactions [4]. One of the attractive approaches to modeling contaminant transport over long time scales as relevant to radionuclide transport, is random-walk particle tracking. The appealing characteristics of this method from a computational standpoint is that it grid independent and simple to parallelize. Moreover, particle tracking methods do not suffer from the numerical dispersion effects of grid based methods when dealing with advection dominated problems [5,6].

Various approaches to particle tracking for transport in fractures have been developed [4,7–9], some of which account for fracture–matrix interactions [4,10–13]. The most efficient of these approaches typically track particles based on the residence time distributions of particles in individual fractures: the time-domain random walk (TDRW) approach of Bodin [10] assumes planar fractures with uniform velocity within each fracture, and the particle residence time in a fracture–matrix unit is calculated from the analytical solution of Maloszewski and Zuber [14] for a linear fracture. The Lagrangian approach of Cvetkovic et al. [4] accounts for spatial variability in velocity field within fractures, and is based on single fracture-scale retention functions whose form was derived from numerical simulations [11]. The residence time distributions involved in the above approaches implicitly assume that fracture–matrix exchange is one-dimensional and perpendicular to the fracture–matrix interface, or that particles are always advected along the same streamline during their transport through a particular fracture. While these are reasonable approximations in light of the other significant uncertainties and complexities in modeling transport through fractured rock, they do not account for some of the transport mechanisms supported by field evidence [15] such as transverse diffusion from preferential flow channels into stagnant or low flow regions in the fracture followed by matrix diffusion from these stagnant regions, or transfer of particles across streamlines following multi-dimensional diffusion within the rock matrix. As noted by Neretnieks [15], some of these processes become particularly important over the long time scales relevant to nuclear waste repositories. Addressing these mechanisms would require very high resolution representations of variable velocity fields (including preferential flow paths and almost stagnant regions) within individual fractures that form part of a large complex fracture network, transverse diffusion normal to streamlines within fractures, fracture–matrix exchange and multi-dimensional models of transport within matrix blocks. DFN flow and transport simulators with such high resolution are under active development [4,16–18].

In this paper, we present an efficient approach for modeling fracture–matrix exchange, which can serve as a component of particle-tracking algorithms in high-resolution DFN flow and transport models. Our approach is based on local-scale analytical solutions to the transport equations in the direction perpendicular to the fracture plane. In contrast to TDRW methods, whose efficiency is realized primarily in the context of simulating breakthrough curves at specified control planes or fracture endpoints, our method is capable of simulating spatial concentration distributions. To establish the accuracy of our algorithm, we present computations for uniform velocity fields and compare our results with analytical solutions. In future work, the fracture–matrix transfer algorithm will be incorporated into high-resolution particle tracking methods that incorporate the features noted above.

The organization of the paper is as follows. We begin with an overview of a standard approach to particle tracking that we use as a basis of comparison; this method is described in Section 2. We then describe our coarse-scale method

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