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A random walk based methodology for the realistic estimation of radioactivity migration in a porous medium

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ABSTRACT

A model for the migration of radioactivity in a porous medium that optimally combines the best of both the statistical and deterministic approaches is developed. To mimic the fractures and the porous matrix we resort to averaging over random samplings of the fracture length and the branching angle between two consecutive nodes of fractures. For propagation between nodes, certain computational aspects of the deterministic parallel fracture model is adopted.

1. Introduction

The safe disposal of the High Level Waste (HLW) from the nuclear industry is an important component of radioactive waste management. The HLW is vitrified in a glass matrix which is sealed in a container. Then one buries this container in the earth at a depth of 500 m or more in a rocky environment. To assess the radioactivity buildup in case of any accidental leak of the species from the container into the porous rock, one needs a realistic model. There are two avenues to address this problem. The first route is through a deterministic way. Using a simplified picture, the rock is considered as an infinite array of parallel fractures separated by porous matrices (Fig. 1). This model was first introduced by Sudicky and Frind (1982). Chen and Li (1997) improved this model further by giving separate labels to the waste matrix and the fracture medium and then enforcing an appropriate inlet source condition. In their description, the migration is described by a set of coupled partial differential equations (pde). When the source is of constant strength, one can solve these equations analytically using Laplace transform techniques (Chen and Li, 1997) and then arrive at the solution as a two dimensional integral. The highly oscillatory nature of the integrand of this solution places a restriction on the maximum distance of evaluation. Due to this complication, in a series of papers we solved these pdes directly by a variety of techniques involving finite difference and pseudospectral methods (Mohankumar, 2007; Sen and Mohankumar, 2011, 2012).

The second route is through a probabilistic estimation. The schematic picture of a rock is given in Fig. 2. We first outline the stochastic model of Williams (1992, 1993) that is based on the analogy with neutron transport in a non-multiplying medium. He assumes that the flow through a fracture can change direction only at a node, the intersection of two or more fractures. The linear distance between two consecutive nodes is the fracture length that is also assumed to be a constant throughout the medium. Smidts and Devooght (1998) developed a methodology using the concept of non-analog Monte Carlo simulation. Giacobbo and Patelli (2008) assumed that the random walk of a particle in a phase space was characterized by two quantities, the free flight kernel and the collision kernel that indicated a transition in the physical–chemical state of a particle (e.g. a contaminant particle meeting a fracture node). Their model and that of Williams (1992) gave identical results for a set of problems (Giacobbo and Patelli, 2008). But these probabilistic models mainly address the migration of radioactive species through a set of interconnected fractures. The drawback of these approaches is that the effect of the porous blocks sandwiched between the interconnected fractures is not taken into consideration. Giacobbo and Patelli (2008) made an attempt to address this issue by assuming a constant adsorption and desorption rate. Cvetkovic et al. (2002) developed a probabilistic method in which the transport of the contaminant particle through a fracture was considered to be a function of advection alone and they ignored diffusion. They incorporated the effect of the porous matrix in the model and assumed that the width of a fracture and the velocity of pore water varied randomly. The statistical estimation of these parameters yielded the escape probability of a radionuclide from a rock. In our present work, we resort to a practical

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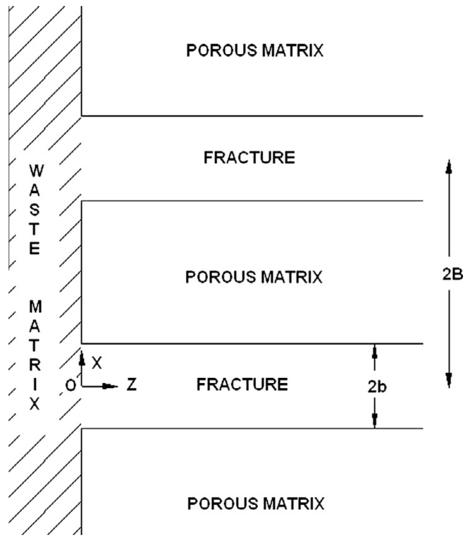

Fig. 1. Parallel fracture model of Chen and Li.

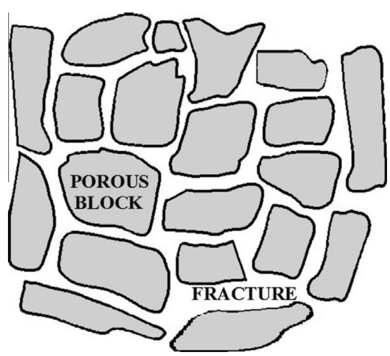

Fig. 2. Schematic picture of a rock.

methodology based on a probabilistic estimation for the evaluation of radioactivity transport in a dual porous medium (porous matrix and fracture). It is known that the actual migration length through a number of interconnected fractures is a random variable. As a first step, this needs to be averaged realistically. Further, the effect of the porous blocks is also to be incorporated in the simulation. For this purpose, we adopt some aspects of the deterministic parallel fracture model of Chen and Li (1997) in the following way. First we replace the linear fracture by this averaged length. Then the diffusion within the porous blocks is taken care of by considering a parametrically varied width of the porous matrix. By resorting to these measures, we hope to capture the random structural details of rock medium in a computationally feasible way.

2. The model

Throughout we assume that the fractures and the porous matrices are uniformly distributed in space (the density of fractures does not change with position). Also we employ meter as the unit of length. The estimation of the average migration length and the effective width of the porous matrices is implemented in two stages. The first stage consists of the generation of a random path between the source and the observation point and like Williams (1992) we assume that the flow in the fractured medium can be described as a series of linear movements that change direction at each node (Fig. 2). By this it is implied that between any two nodes there is no change in the direction of the flow. Cvetkovic et al. (2002) allowed the fracture length to vary uniformly between 1 and 10 and hence we let the fracture length lie in the interval [1, 10]. The randomly oriented fracture lengths between two nodes are sampled from this range. Moreover, following Giacobbo and Patelli (2008) it is assumed that at each node the orientation of the fractures is uniformly distributed between ϕ_{max} and $(-\phi_{max})$ with respect to the mean flow direction. This angle describing the orientation of the new fracture is called the branching angle. By randomly sampling the fracture length and the branching angle we generate an *average migration length* between the source and the observation point by the following steps.

I. Sample the fracture length between two consecutive nodes from a uniform distribution in [1, 10].
II. Sample the branching angle.
III. A fracture of length L_f oriented at an angle ϕ has a projection of magnitude $L_f\,cos(\phi)$ in the mean flow direction. So to cover a linear distance (L_{SD}) along this direction between the source and the observation point, one has to repeat steps I and II till the quantity $\left(\sum_{i=1}^{N} L_f^i\ cos(\phi^i)\right)$ equals L_{SD}.
IV. Steps I–III give *a value* for the migration length. Repeat this for a number of times to get an *average migration length* between the source and the observation point.

The second stage is the estimation of the average width of porous matrix. It is very difficult to model the migration of contaminant particles in a medium with dual porosity if one is restricted to the domain of probabilistic methods like Monte Carlo. The model of Williams (1992, 1993) has no allowance for the migration through the porous blocks. Giacobbo and Patelli (2008) tried to address this issue (the effect of porous blocks) by assuming a constant adsorption and desorption rate. But in reality the diffusion rate within a porous block depends on the concentration of the contaminant particle at a particular location at a particular instant of time. This key point is taken care of in the deterministic parallel fracture model of Chen and Li (1997). Here we try to implement this ingredient as practically as possible and an important ingredient for this aspect is the width of the porous matrix. It is very difficult to find the average of this truly random variable. So in our model we parametrise this quantity as follows. Let $L_{f,max}$ and ϕ_{max} denote the maximum length of a fracture and the branching angle respectively. Then the maximum distance of separation between two consecutive fractures takes a value $\Delta = 2L_{f,max}sin\phi_{max}$ while the minimum separation distance is zero (at a node). So the average width of the porous matrix falls within the interval [0,Δ]. Uniformly spaced points in this interval are chosen as representative magnitude of the width of the porous matrix.

Below we briefly describe the deterministic parallel fracture model of Chen and Li. In this approach the rock is considered as an assembly of infinite array of parallel fractures of equal width (2b) and they are separated by porous matrices (Fig. 1). The width of the porous matrix is taken as 2B. We denote the distance along the fracture by z and assume that the point $z = 0$ separates the waste matrix and the fracture. The transverse direction is represented by x. Let $C(z,t)$ and $C_p(x,z,t)$ be the concentrations of the active species in the fracture and in the porous matrix, respectively. The flow of the contaminant particles is expressed by the following pdes.

$$\frac{\partial C_p}{\partial t} - \frac{D_p}{R_p}\frac{\partial^2 C_p}{\partial x^2} + \lambda C_p = 0; \quad b \leqslant x \leqslant B; \quad t \geqslant 0 \tag{1}$$

$$\frac{\partial C}{\partial t} + \frac{v}{R}\frac{\partial C}{\partial z} - \frac{D}{R}\frac{\partial^2 C}{\partial z^2} + \lambda C + \frac{q}{Rb} = 0; \quad z \geqslant 0; \quad t \geqslant 0 \tag{2}$$