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EFFECTIVE SOLUTE TRANSPORT WITH LINEAR SORPTION IN LATTICE FRACTURE NETWORKS

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Summary.

We study transport in a lattice fracture network with uncorrelated velocity fields using a stochastic modeling approach. We consider a two-dimensional regular fracture network model characterized by a constant fracture length and fracture angle. The transport velocity in the fractures is a random variable. Here, we present an exact derivation of effective equations for the average particle density and concentration variance from the microscopic disorder model. Within a Lagrangian transport framework, we derive effective equations for particle transport by coarse graining, noise averaging and ensemble averaging of the local scale Langevin equations. We rigorously show that average particle density describes effectively an uncoupled continuous time random walk (CTRW) and the concentration variance is quantified by a two particle CTRW. The obtained mean behavior and concentration variance are compared to direct numerical simulations of particle transport in single medium realizations and the corresponding ensemble averages.

1 INTRODUCTION

Understanding flow through fractures is essential for improving several societal related issues, including the risk assessment of nuclear waste disposal [1,2], the site selection and assessment of leakage risk in geological CO2 storage [3], the oil and gas production from fractured carbonates [4, 5], and the development of enhanced geothermal systems [6]. There are two key obstacles to predicting transport through fractured media. The fundamental challenge is that the location and properties of individual fractures are not identifiable. At best, only some representative properties of the network can be inferred from analogue geologic outcrops or high-resolution seismic interpretation [7, 8]. Second, it is well known that flow through fractures leads to anomalous transport [9, 10]. Anomalous transport refers to the spreading of a

substance or a signal in a way that deviates from classical diffusion and cannot be accurately captured with traditional advection diffusion equation. Due to these reasons, predictive capabilities related to real fractured and heterogeneous media are severely limited. Anomalous transport is not only limited to fluid flow. It is also observed in many other transport phenomena such as heat and light diffusion [11], the distribution of human travel [12] and the occurrence of earthquakes [13]. In this work, we develop a stochastic framework to understand and predict anomalous transport through fractured media. We adopt a Lagrangian viewpoint to develop a macroscopic (effective) description of transport in a simple fracture network model. Recently, a Lagrangian framework was used to upscale unidirectional transport of an adsorbed solute in a chemically heterogeneous medium [14]. In that work, it was shown that the transport through a porous medium with constant hydraulic conductivity and spatially uncorrelated heterogeneous retardation factor follows the CTRW framework. We will generalize the coarse graining and ensemble averaging methodology to the simple 2D fracture network. We show that the transport through a simple lattice fracture networks can be described, exactly, as a CTRW that is parameterized by the local scale medium properties and transport characteristics. We will develop an Eulerian formulation by performing a Kramers-Moyal expansion [15] of the Master equation and derive effective equations for the ensemble mean transport.

2 METHODOLOGY

2.1 Physical setting

We consider a simple fracture network model consisting of two sets of parallel, equidistant, intersecting fractures: one set at an angle $+\alpha$ and the other at an angle $-\alpha$ with respect to the x-axis, embedded in an impermeable matrix (see Fig. 1). The network is then viewed as a regular lattice of nodes and links. The nodes are assumed to be volumeless. The links of the network have spatially-distributed properties. In our fracture model, we assume constant aperture for all links, and a spatially distributed retardation coefficient R. This implies that the flow velocity u through the links of the network is constant, while the effective solute velocity v (flow velocity divided by retardation factor $v = \frac{u}{R}$) is spatially variable. In the case of mass transport accompanied by linear sorption, the retardation factor R is defined as $R = 1+k$, where k is a dimensionless sorption coefficient. The network is random in the sense that the retardation coefficient at each link of the network is drawn from a given statistical distribution. Numerous studies at various scales and in different sites have shown that the distribution of many fracture properties often follows a power-law. In nature the power laws have to be limited by the upper or lower limits to the scale range over which they are valid [7]. Therefore, we assumed a truncated power-law distribution for k, $p_k = N\frac{1}{k^{1+\beta}}\exp(-\frac{1}{k})$, where N is normalization factor and β is a parameter defining the slope of the power law (Fig. 1). We generate ensemble of the fracture network realizations using same p_k for each realization. The set of all realizations generated in this way form a statistical ensemble that is stationary and ergodic.

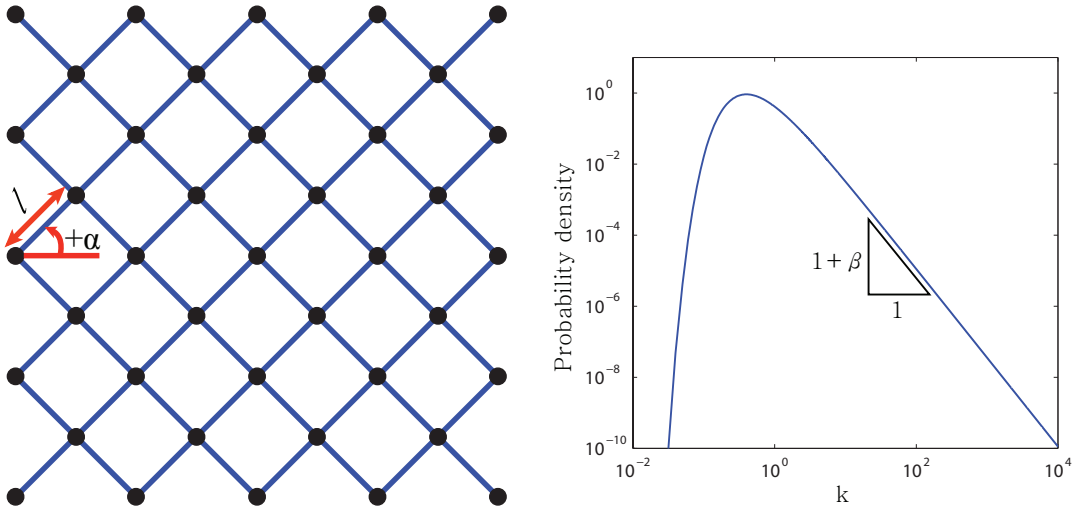

Figure 1: A simple fracture network with the constant fracture length (l) and two sets of fracture orientation $\{-\alpha, +\alpha\}$ with respect to x-axis (left) and the truncated power law distribution of a dimensionless sorption coefficient (k) with $\beta = 1.5$ (right)

2.2 Monte Carlo simulations

Solute transport through our lattice fracture system can be described in terms of Lagrangian equations. Let $\mathbf{x}(t) = [x(t), y(t)]^T$ be the solute particle position at time t. Its evolution with time t is given by

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = v[\mathbf{x}(t)]\cos\{\theta[\mathbf{x}(t)]\}, \qquad \frac{\mathrm{d}y(t)}{\mathrm{d}t} = v[\mathbf{x}(t)]\sin\{\theta[\mathbf{x}(t)]\}, \tag{1}$$

where $\theta \in \{-\alpha, +\alpha\}$ is the fracture orientation and v is the particle velocity, which varies from fracture to fracture. We rewrite this system of Langevin equations using a time parameterization $t(s)$:

$$\frac{\mathrm{d}x(s)}{\mathrm{d}s} = \cos\{\theta[\mathbf{x}(s)]\}, \qquad \frac{\mathrm{d}y(s)}{\mathrm{d}s} = \sin\{\theta[\mathbf{x}(s)]\}, \tag{2a}$$

and

$$\frac{\mathrm{d}t(s)}{\mathrm{d}s} = \frac{1}{v[\mathbf{x}(s)]}, \tag{2b}$$

where the random walk $\mathbf{x}(t)$ is parameterized in terms of a continuous variable s, which has a meaning of operational time: the process $s(t)$ is a continuum analog of the number of steps $n(t)$.

The time evolution of solute particle takes place on a regular lattice with constant fracture length l and fracture orientations $\{-\alpha, +\alpha\}$. At each joint, the particle can enter either of the

two fractures with equal probability. Thus, the above set of Langevin equations can be coarse grained by setting $\Delta s = l$, which yields the discrete equations:

$$x_{n+1} = x_n + l\cos(\alpha), \qquad y_{n+1} = y_n + \xi_n l\sin(\alpha), \tag{3a}$$

and

$$t_{n+1} = t_n + \frac{l}{v_n}, \tag{3b}$$

where $\xi \in \{-1, +1\}$ represents an equiprobability random process $p_\xi = \frac{1}{2}\delta(\xi+1) + \frac{1}{2}\delta(\xi-1)$, assumed to be uncorrelated in time and space. We solve the transport problem by numerical random walk simulations using (3), for many realizations of the random network. We assume a point source at origin as an intial condition. In other words, all the particles are released at $\mathbf{x} = 0, t = 0$. The concentration is defined as number of particles at each node divided by the total number of particles and the area represented by the joint. In each realization, the transition time from node to node depends on the position of the particle. The simulated concentration field is highly variable from realization to realization due to differences in the particle velocity field, as can be seen in Figure 2. We will show, however, that by averaging over all possible realizations, the transition time becomes independent of particle position as long as the underlying random field is statistically stationary.

2.3 Derivation of ensemble mean concentration

The particle distribution $c(\mathbf{x}, t)$ in a single realization is given by

$$c(\mathbf{x}, t) = \langle \delta \left\{ \mathbf{x} - \mathbf{x}[s(t)] \right\} \rangle , \tag{4}$$

where δ denotes the Dirac delta distribution, and the angular brackets denote white-noise average over many solute particles. The ensemble average of the particle distribution over realizations (i.e., the ensemble mean concentration) is given by

$$\bar{c}(\mathbf{x}, t) = \overline{\langle \delta \left\{ \mathbf{x} - \mathbf{x}[s(t)] \right\} \rangle}, \tag{5}$$

where the overbar denotes the ensemble average over realizations. If we assume point injection as an initial condition, the probability of a particle being at a certain position after a fixed number of jumps is the same for all realizations because the topology of the fracture network is fixed, and we assumed equal probability of jumping upward and downward at each joint. Moreover, the particle position and transition time are independent after ensemble averaging because the spatial distribution of the retardation factor is obtained from the same probability distribution for all realizations. Using these facts we can prove that the ensemble space-time transition probability density follows,

$$\overline{\langle \delta \left[(\mathbf{x} - \mathbf{x}') - \Delta\mathbf{x} \right] \delta \left[(t - t') - \Delta t \right] \rangle} = \eta(\mathbf{x} - \mathbf{x}')\psi(t - t'), \tag{6}$$

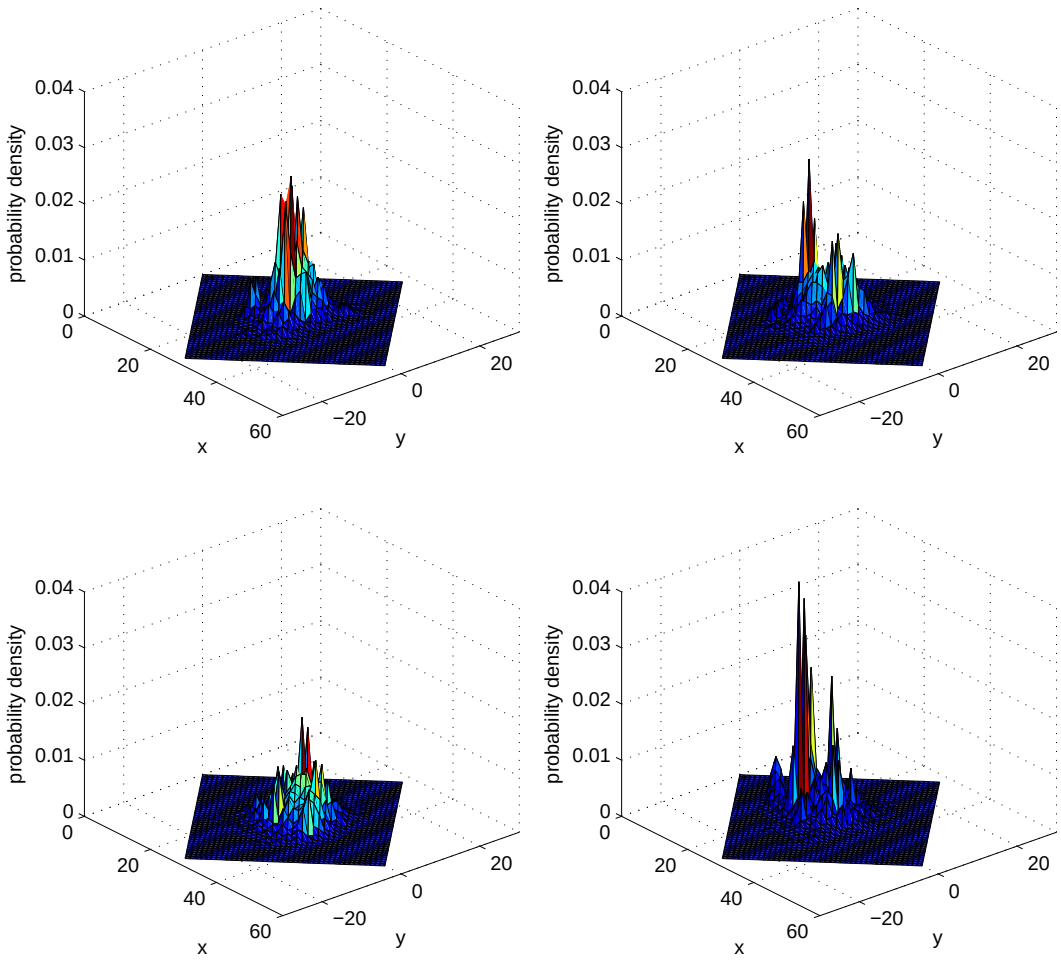

Figure 2: Mean concentration obtained by numerical random work simulations over four different velocity fields. Each velocity field was generated from the same probability density distribution and the result shows the large variability of the mean concentration.

where $\eta(\mathbf{x}-\mathbf{x}') \equiv \langle \delta[(\mathbf{x}-\mathbf{x}')-\Delta\mathbf{x}]\rangle$ is the spatial transition probability density between two adjacent nodes ($\mathbf{x}'$ and $\mathbf{x}$), and $\psi(t-t')$ is the corresponding temporal transition (jumping-time) probability density. In our fracture model, spatial transition probability density becomes $\eta(\mathbf{x}-\mathbf{x}') = \delta[x-(x'+lcos\theta_0)]\left\{\frac{1}{2}\delta[y-(y'+l\sin\alpha)]+\frac{1}{2}\delta[y-(y'-l\sin\alpha)]\right\}$, and the temporal transition probability density becomes $\psi(t-t') = \frac{1}{l}p_k(\frac{t-t'}{l}-1)$. Equation (6) is our fundamental result: the transition distance probability and transition time probability are independent, and each depends only on the distance between nodes and transition time. We conclude that our lattice fracture model with heterogeneous sorption can be represented exactly by uncorrelated Continuous Time Random Walk (CTRW) model [15, 16].
Using the transition distance probability and transition time probability, we showed in the Appendix that the ensemble mean concentration can be defined as following.

$$\bar{c}(\mathbf{x},t) = \int_0^t dt' \left[1-\int_0^{t-t'} d\tau\psi(\tau)\right] R(\mathbf{x},t'), \tag{7a}$$

and

$$R(\mathbf{x},t) = P_0(\mathbf{x},t) + \int_\Omega d\mathbf{x}' \int_0^t dt'\eta(\mathbf{x}-\mathbf{x}')\psi(t-t')R(\mathbf{x}',t'), \tag{7b}$$

where $P_N(\mathbf{x},t) \equiv \overline{\langle\delta(\mathbf{x}-\mathbf{x}_N)\delta(t-t_N)\rangle}$ is the probability density of a particle arriving at position $\mathbf{x}$ at time t after n steps, and $R(\mathbf{x},t) \equiv \sum_{N=0}^{\infty} P_N(\mathbf{x},t)$ is the probability density for a particle to just arrive at position $\mathbf{x}$ at time t. Accordingly, $P_0(\mathbf{x},t) = \delta(\mathbf{x}-\underline{0})\delta(t-0)$ is the space-time particle distribution after 0 steps, which denotes a pulse point injection of all particles at the origin. If we introduce a median transition time t_1, the transition velocity $\mathbf{v} = \frac{\bar{\mathbf{x}}}{t_1}$ and the dispersion tensor $\mathbf{D} = \frac{\overline{\mathbf{x}^2}}{2t_1}$, the partial differential equation (PDE) form of (7) can be obtained using Laplace transform and Taylor expansion [17].

$$s\bar{c}^*(\mathbf{x},s) = \delta(\mathbf{x}-\underline{0}) - \mathbf{v}\cdot[\nabla\bar{c}^*(\mathbf{x},s)]M^*(s) + \mathbf{D}:[\nabla\nabla\bar{c}^*(\mathbf{x},s)]M^*(s), \tag{8}$$

where the star superscript (*) denotes the Laplace-transformed variable and s is the Laplace variable. Laplace-transform of memory function $(M^*(s))$, the first moment of $\eta(\mathbf{x})$ $(\bar{\mathbf{x}})$ and the second moment of $\eta(\mathbf{x})$ $\left(\overline{\mathbf{x}^2}\right)$ are defined as,

$$M^*(s) = \frac{st_1\psi^*(s)}{1-\psi^*(s)} \tag{9}$$

$$\bar{\mathbf{x}} = \int d\mathbf{x}'\eta(\mathbf{x}')\mathbf{x}' \qquad\qquad \overline{\mathbf{x}^2} = \int d\mathbf{x}'\mathbf{x}'\otimes\mathbf{x}'\eta(\mathbf{x}'). \tag{10}$$

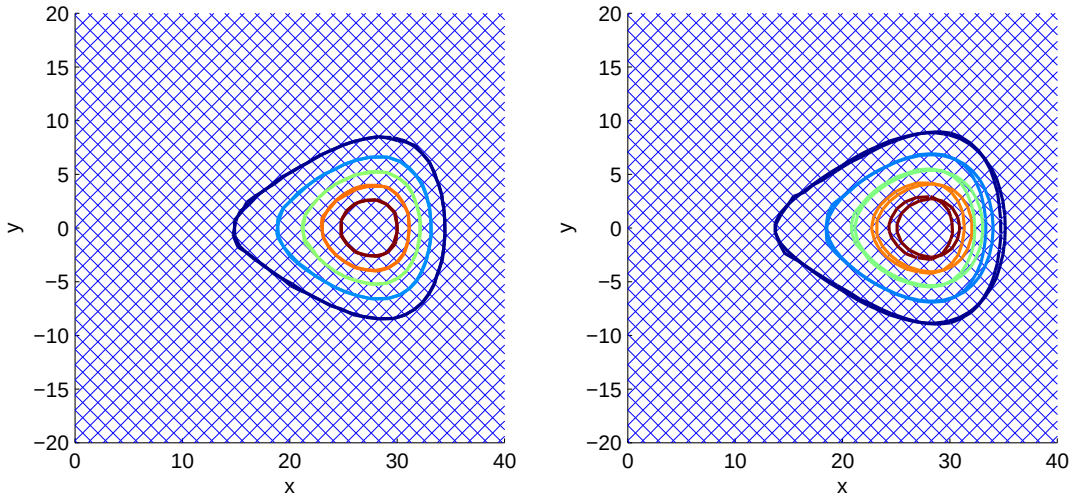

Figure 3: Comparison of ensemble mean concentration obtained from Monte Carlo simulation over 10000 realizations and uncorrelated CTRW simulation (left) and Comparison of ensemble mean concentration of Monte Carlo simulation over 10000 realizations and Analytical solution obtained by solving PDE form of CTRW equation.

For our fracture model, $\bar{\mathbf{x}} = (\overline{x_1}, \overline{x_2}) = (lcos\theta_0, 0)$ and $\overline{\mathbf{x}^2} = \begin{pmatrix} \overline{x_1 x_1} & \overline{x_1 x_2} \\ \overline{x_2 x_1} & \overline{x_2 x_2} \end{pmatrix} = \begin{pmatrix} (lcos\theta_0)^2 & 0 \\ 0 & (lsin\theta_0)^2 \end{pmatrix}$ which is showen in the Appendix. Now apply inverse Lapace transform to (8), and we can get

$$\frac{\partial}{\partial t}\bar{c}(\mathbf{x}, t) = -\int_0^t M(t - t') \left[\mathbf{v} \cdot \nabla \bar{c}(\mathbf{x}, t') - \mathbf{D} : \nabla\nabla \bar{c}(\mathbf{x}, t')\right] dt' \tag{11}$$

We verified our results by comparing ensemble mean concentration obtained from three different methods.

1. Ensemble averaging of Monte Carlo particle tracking simulations over 10000 realizations using the Langevin equation given in (3).

2. Uncorrelated CTRW particle tracking simulation with Langevin equation using uncorrelated space-time transition proability given in (6).

3. Solving (8) using inverse Laplace transform.

Figure 3 shows that all three methods provide almost identical ensemble mean concentration. The plot on the left of Figure 3 shows that the uncorrelated CTRW particle tracking simulation and the ensemble averaging of the Monte Carlo simulations are exactly identical. This verifies that the transport through our fracture model follows uncorrelated CTRW. Moreover, this is numerically significant result since this implies that we can obtain ensemble mean concentration with less computational expanse compared to ensemble averaging of Monte Carlo simulations. The plot on the right of Figure 3 is almost identical, but we can notice slight difference of the plume front shape. This may be caused by numerical Laplace inversion. However,

the difference is negligible and we can conclude that our effective equation (11) gives exact solution. The developed model accurately captured anomalous transport and, most importantly, the plume shape and the evolution are determined only by one parameter (β) which is the slope of the power law region. As a result, this model is also highly efficient for the parameter determination using inversion.

3 CONCLUSIONS

The significance of this work is that the macroscopic effective transport behavior has been derived directly from the small scale fracture description. It turns out that such macroscopic description takes the form of an uncorrelated CTRW. The description relies solely on the particle jumping time distribution, which depends -in our model- on a single parameter. The plume shape and evolution was dictated by β. However, it is important to note that the CTRW model provides ensemble mean concentration which is not an exact mean concentration for a specific realization. Therefore, information about variance between realizations is important for understanding variability. Ensemble mean together with variance will provide essential information for the quantification of effective transport in fractured media. However, most physical systems require the transport velocities to be correlated. Therefore, we will try to generalize our model for the correlated velocity field for the future work. We conjecture that the effective transport model may take the form of a correlated CTRW if the Lagrangian velocity is a spatial Markov process [18]. We will try to apply our methodology to correlated velocity field and check the applicability of correlated CTRW.

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