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Comment on "Flow and Tracer Transport in a Single Fracture: A Stochastic Model and Its Relation to Some Field Observations" by L. Moreno et al.

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Moreno et al. [1988] (hereinafter referred to as MT) used a particle-tracking scheme to investigate the physics of solute movement in a variable-aperture planar fracture. The spatially heterogeneous fluid velocity was assumed to be the only mechanism of solute movement; local or pore scale dispersion and molecular diffusion were assumed to be negligible. The particle-tracking scheme used by MT consisted of routing particles from node to node in a finite difference grid. In this scheme, the direction of an individual particle is randomly selected and the probability associated with the particle movement in a given direction is proportional to the fluid flux in that direction. The same method was used by *Desbarats* [1990] to investigate advective transport in aquifers composed of two porous media of different hydraulic conductivities.

The node-to-node routing scheme used by MT is a poor model of the physics of advective solute movement in a continuum. In a companion comment [*Goode and Shapiro*, this issue], we analyze the artificial dispersion introduced by this scheme for the case of uniform flow. Those results are directly applicable to the discussion here. In this comment we show the smearing effect of the node-to-node routing scheme on particle breakthrough, and we show that the spreading indicated by the "transfer matrix" analysis proposed by MT is solely an artifact of the node-to-node routing scheme. The differences in particle breakthrough presented here between the node-to-node routing scheme and a linear velocity interpolation method are indicative of the differences for binary porous media as considered by *Desbarats* [1990].

Our comments focus only on the errors introduced in employing the node-to-node routing scheme and its impact on simulating advection-dominated solute movement. We do not comment on the conclusions reached by MT with regard to the physics of their problem. Use of a model that accurately treats advection-dominated solute movement may or may not influence the conclusions of these investigators; however, we believe that there are more appropriate and available models that can be used to investigate advection-dominated solute movement.

Node-to-Node Routing in a Variable-Aperture Fracture

MT applied the node-to-node routing scheme to advective solute transport in a single planar fracture. MT (p. 2037) described the method as follows: "Particles coming to an intersection as distributed in the outlet branches with a probability proportional to the flow rates. The residence time for the particle to reside within each square element is determined from the flow rate through this element and the volume involved .... " The only physical process under study was the advection of solute. MT continued, "In this calculation, we focus on the effects of the different residence times along the different pathways as the chief source of the overall dispersion in the fracture. We therefore do not include the effects of molecular diffusion, matrix diffusion or local dispersion within each channel in our calculations." In MT's work, the nodes are located at the center of the blocks and the aperture is considered to be constant over the block, which leads to the use of harmonic means for interblock conductances. The "outlet branches" are the lines connecting nodes; hence each line has a residence time associated with it that is determined by adding the residence times within the two segments of the line, one segment in each block. The residence time within each block is defined by equation (11) of MT:

$$t_i = \frac{b_i \Delta x \Delta y}{\frac{1}{2} \sum_j |Q_{ij}|}$$

where b_i is the aperture of the block, Δx and Δy are the block dimensions, and $|Q_{ij}|$ is the absolute value of the volumetric flux from node i to node j.

This formulation only allows movement along the lines connecting nodes, which may be appropriate when these lines are the discrete fractures of a network [*Schwartz et al.*, 1983]. However, this formulation introduces errors when applied to the continuum of a single planar fracture. As pointed out by *Schwartz et al.* [1983, p. 1256], "Built into this scheme for partitioning mass at the intersections is the assumption that there is perfect mixing at the fracture intersections." In the case of MT, the "fracture intersections" are nodes; hence perfect mixing occurs at each node in the model. Thus, local artificial dispersion is introduced in the model solely as an artifact of the particle-tracking scheme.

To illustrate the errors induced by application of the node-to-node routing scheme of MT to a single fracture, a two-dimensional problem is considered that generally corresponds to simulations conducted by MT where block average fracture apertures are generated stochastically. The aperture is a lognormally distributed random variable, Y, where $Y = \log_{10} b$ and b is the fracture aperture in micrometers. The mean and variance of Y are $E[Y] = 1.7$ and $\sigma_Y^2 = E[YY] - (E[Y])^2 = (0.43)^2$, respectively. In addition, Y is

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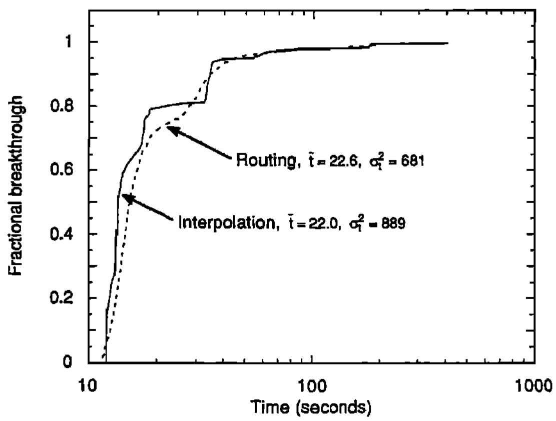

Fig. 1. Fractional breakthrough for 1000 particles in a variable-aperture planar fracture using node-to-node routing and velocity interpolation. The mean ($\bar{t}$) and variance (σ_t^2) of breakthrough time are shown for both methods.

assumed to have a negative exponential and isotropic covariance function,

$$R(r) = \sigma_Y^2 \exp\left(\frac{-|r|}{\Lambda}\right) \tag{1}$$

where R is the covariance, r is the separation distance, and the correlation length, $\Lambda = 0.25$ m. A single realization of block average apertures is generated using the turning bands method [*Mantoglou and Wilson*, 1982; *Zimmerman and Wilson*, 1989] for a 21 (x) by 20 (y) grid having $\Delta x = \Delta y = 0.05$ m.

Solute advection in this variable-aperture fracture is simulated using both an implementation of the node-to-node routing scheme of MT and a linear velocity interpolation method [*Goode*, 1987, 1990]. Linear and other velocity interpolation methods treat the flow system as a continuum and move particles throughout the domain by computing the velocity at any point in the domain. Each separate particle follows a unique deterministic path corresponding to a streamline in steady flow. These methods have been used extensively to simulate advection in groundwater flow systems [e.g., *Reddell and Sunada*, 1970; *Konikow and Bredehoeft*, 1978; *Prickett et al.*, 1981]. The linear velocity interpolation method yields exact solutions for advection-only transport for the case of uniform flow, regardless of orientation of the grid [*Goode and Shapiro*, this issue]. A planar fracture is a continuous domain in two dimensions and velocity interpolation methods can be applied to this physical system without difficulty.

No-flow boundary conditions are assumed on the top ($y = 10$ m) and bottom ($y = 0$ m) borders of the grid. Fixed head boundaries are applied at nodes along the left ($x = 0.025$ m) and right ($x = 10.025$ m) borders to yield a mean velocity in the positive x direction. Particles are released at the nodes in column 2 ($x = 0.075$ m) of the grid and the number of particles released in each block is proportional to the flux leaving the block in the x direction. For the linear velocity interpolation method, particles are initially spread evenly in the y direction within each block. Figure 1 shows the breakthrough of 1000 particles at $x = 1$ m using the node-to-node routing scheme and using linear velocity interpolation. The breakthrough for the routing scheme is smoother due to

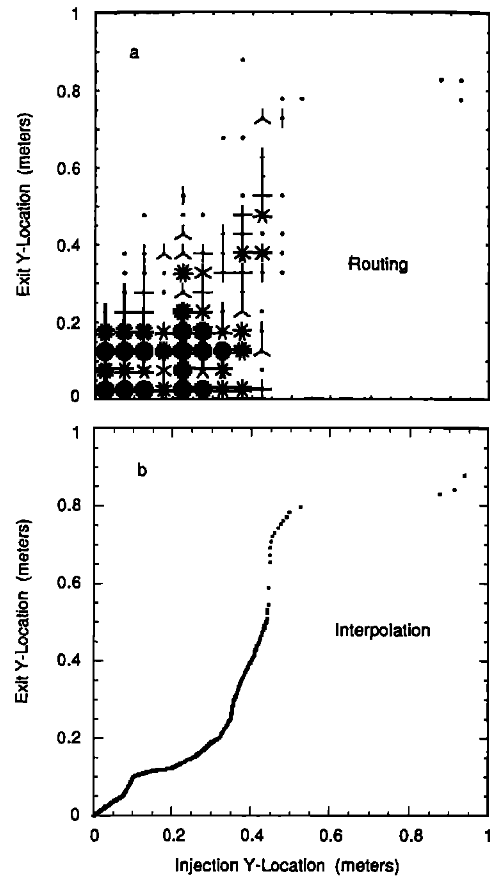

Fig. 2. Exit y location as a function of injection y location for 1000 particles in a variable-aperture planar fracture using (a) node-to-node routing and (b) velocity interpolation. In Figure 2a, the number of particles for each node location pair is indicated by the number of petals on the "flower." A single point indicates only one particle for that node location pair.

the artificial dispersion that is introduced. The total residence time of most particles is overestimated using the node-to-node routing scheme. This particular simulation exhibits about 8% difference in the mean residence time. The mean ($\bar{t}$) and variance (σ_t^2) of the residence time for both methods are strongly influenced by the extremely long residence times of a few particles.

MT proposed the transfer matrix plot (MT, Figures 8–11) to show the relation between the y location on the injection face and the y location on the exit face of all particles. For example, MT's Figure 8 (bottom right) shows that most particles were injected at $y = 0.575$ m and that these particles left the system primarily at $y = 0.275$ m, $y = 0.425$ m, and $y = 0.625$ m. In addition, particles injected at $y = 0.725$ m exited primarily at $y = 0.425$ m and $y = 0.625$ m. These results indicate that particles are mixing across streamlines. In the absence of local dispersion, particles should not cross streamlines and the exit y location should be a monotonically increasing function of the injection y location. All particles injected at $y = 0.725$ m should exit the system at a y location greater than the y location exit for particles injected at 0.575 m, or injected at any $y < 0.725$ m.

Figure 2 shows the particle exit y location as a function of each particle's injection y location for the node-to-node routing scheme (Figure 2a) and for particle-tracking with linear velocity interpolation (Figure 2*b*). These results are for the same simulation used to generate Figure 1. Instead of contouring the results for the routing scheme as done by MT, Figure 2*a* shows the particle density for each injection-exit node *y* location pair by the number of petals on the "flower." A single point indicates only one particle at that *y* location pair. This representation, or contouring, is required in part because many particles may have the exact same position due to the discrete nature of the node-to-node routing scheme. Figure 2*a* corresponds to the "transfer matrix" plots of MT. Figure 2*b* shows the injection and exit *y* locations of each particle for the interpolation method which yields the expected monotonically increasing relation. In the results presented by MT, the spread in the "transfer matrix" was entirely due to the artificial dispersion introduced by the node-to-node routing scheme, and was not related to the physical properties of the fractures.

Conclusions

The numerical model used by MT to simulate advective transport in a variable-aperture planar fracture introduced artificial dispersion that was not included in the conceptual model under which the results were interpreted. Whether or not the "transfer matrix" analysis proposed by MT has value in real experiments, the spreading in the numerical results shown by MT was an artifact of the node-to-node routing scheme. Particle-tracking methods that do not introduce artificial dispersion are available and can be applied to MT's problem without difficulty. We hope that this discussion will contribute to the use of appropriate methods for simulation of advective transport in heterogeneous flow regimes.

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