

Finite Difference Modeling for Scale-Dependent Dispersivity in a Fractured Medium

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Abstract

A new finite difference model is developed for solute transport in a fractured medium that can consider advection, adsorption, first-order decay, and scale-dependent dispersivity of individual fractures. In the model, the dispersivity of individual fractures is employed as a variable increasing with travel distance from a source. The model is verified using an analytical solution for a single fracture. A solution from the new model is independent of the outlet boundary condition of fractures, and has little numerical dispersion error.

key word : scale-dependent dispersivity, finite difference method, fracture network.

1. Introduction

A single fracture is a basic model for the simulation of solute transport in a fractured medium. Many previous field studies show that dispersivity of a single fracture increases with fracture length because of the heterogeneity of fracture aperture distributions (Raven *et al.*, 1988; Cady *et al.*, 1993). In this study, a new finite difference model is developed for solute transport in a fractured medium that can consider advection, adsorption, first-order decay, and the scale-dependent dispersivity of individual fractures. The dispersivity is simulated as a variable increasing with travel distance from a source.

2. Development of a Solute Transport Model

If one assumes that hydraulic dispersion coefficient in a fracture is dependent on the travel distance from a source, the transport of solutes in a single fracture including a linear equilibrium isotherm and first-order decay can be written as (Yates, 1990)

$$\frac{\partial c}{\partial t} + \frac{v_f}{R_f} \frac{\partial c}{\partial x} - \frac{1}{R_f} \frac{\partial}{\partial x} \left(D_f(x) \frac{\partial c}{\partial x} \right) + \mu c = 0 \quad (1)$$

$$D_f(x) = \alpha_f(x) v_f + D^*, \quad R_f = 1 + \frac{K_f}{b_{1/2}}$$

where c is the concentration of solutes in solution, t is the time, v_f is the fluid velocity

in the fracture, R_f is the retardation factor in the fracture, x is the coordinate along the fracture axis, $D_f(x)$ is the hydraulic dispersion coefficient in the fracture, μ is the decay constant, $\alpha_f(x)$ is the dispersivity of the fracture, D^* is the molecular diffusion coefficient, K_f is the distribution coefficient in the fracture, and $2b_{1/2}$ is the fracture aperture. The $\alpha_f(x)$ can be adequately described using Eq. 2 (Pickens and Grisak, 1981; Yates, 1990).

$$\alpha_f(x) = a_f x \quad (2)$$

where a_f is the slope of dispersivity-distance relationship.

Han *et al.* (2001) developed a finite difference model for solute transport in a single fracture as follows.

$$c_i^{n+1} = \frac{1}{R_f} \left[(1 - \mu R_f \Delta t) c_i^* + \frac{K_f}{b_{1/2}} c_i^n \right] \quad (3)$$

$$c_i^* = \lambda c_{i-1}^n + (1 - \lambda) c_i^n, \quad \lambda = \frac{v_f \Delta t}{\Delta x_f} \quad (4)$$

where c_i^{n+1} is the new time level concentration at transport node i calculated *with* consideration for the adsorption and first-order decay, Δt is the time step, c_i^* is the new time level concentration at transport node i calculated *without* consideration for the adsorption and first-order decay, c_i^n is the old time level concentration at transport node i , λ is the Courant number, and Δx_f is the length between transport nodes. In their model, the dispersivity of a single fracture was simulated artificially by the following equation.

$$\alpha_f = \frac{l_f}{2N_f} \left(1 - \omega \frac{v_f}{l_f} \right) \quad (5)$$

where α_f is the dispersivity of the fracture, l_f is the length of the fracture, $N_f (=l_f/\Delta x_f)$ is the number of transport nodes in the fracture, and $\omega (= \Delta t N_f)$ is the constant related to time step.

Eq. 1 can be solved numerically using Eqs. 3 and 4 with proper transport node allocation. The idea is that a fracture is divided into several sub fractures and the artificial dispersivity of a sub fracture ($\alpha_{f,i}$) is set to be the same with the dispersivity at the center of the sub fracture. In this case, after some algebraic manipulation according to Eqs. 2 and 5 with $1/(2N_{f,i}) = \alpha_{f,i}$,

$$l_{f,i+1} = 3l_{f,i} \quad (i \geq 2) \quad (6)$$

$$l_{f,i} = 2\delta_f, \quad \delta_f = \omega v_f \quad (7)$$

where $N_{f,i}$ is the total number of transport nodes in the i -th sub fracture and $l_{f,i}$ is the length of the i -th sub fracture.

In brief, one can simulate the transport of solutes in a single fracture with travel distance dependent dispersivity using Eqs. 3 and 4, if one divides the fracture into several sub fractures according to Eqs. 6 and 7, and allocates transport nodes whose number is $1/(2\alpha_f)$ per one sub fracture.

3. Verifications and Application of the Model

Yates (1990) obtained the analytical solution for Eq. 1 with the step-function input (c_i) and zero initial concentration assuming that $D_f(x)$ could be described as

$$D_f(x) = \alpha_f(x)v_f + \text{diffusion} = (a_f x + l_f b_f)v_f \quad (8)$$

where l_f is the characteristic distance and b_f is the constant that characterizes the fluid diffusive processes. The developed model is verified using the analytical solution given by Yates (1990). Table 1 shows the input parameters for the analytical solution, and Figure 1 shows transport nodes for the finite difference model developed in this study. δ_f is 12.5 cm, which divides a fracture of 10 m into four sub fractures.

Table 1. Input parameters for the analytical solution to verify the model developed

$2b_{fz}$ (mm)	l_f (m)	a_f	l_f (m)	b_f	v_f (m/day)	c_i (ppm)
0.1	10	0.1	1.0	0.01	0.1	1.0

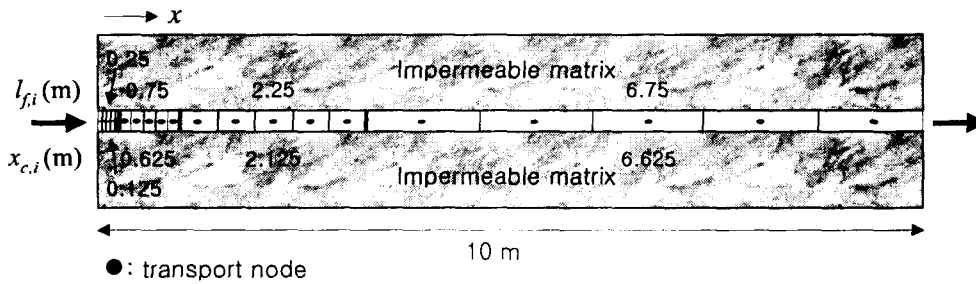


Figure 1. Transport nodes used to verify the developed model.

Figure 2 shows the comparisons of results from the analytical solution and the numerical solution. Although the number of sub fractures is relatively small, one can see that the simulated results are in good agreement with the analytical solution.

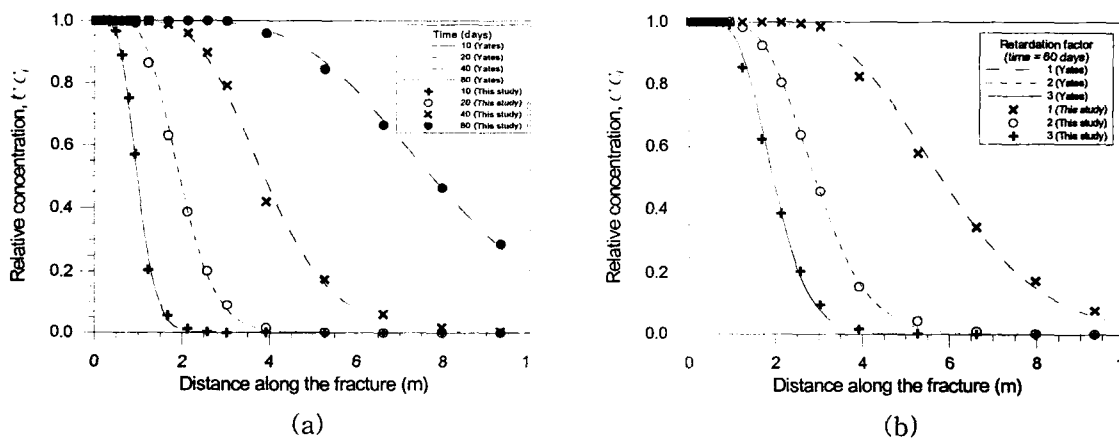


Figure 2. The change of concentration with (a) time and distance (no adsorption, no first-order decay), and (b) retardation and distance (observation time=60 days, no first-order decay).

Considering the scale-dependent dispersivity of individual fractures, the new model is especially suitable for a fractured medium with variable fracture length distributions. An example of the transport nodes in a fractured medium is shown in Figure 3. One can see that the method for transport node allocation not only simulates the scale-dependent dispersivity of an individual fracture, but also enables one to easily know the flowing direction in a fracture because the distance between transport nodes increases in the direction of the flow.

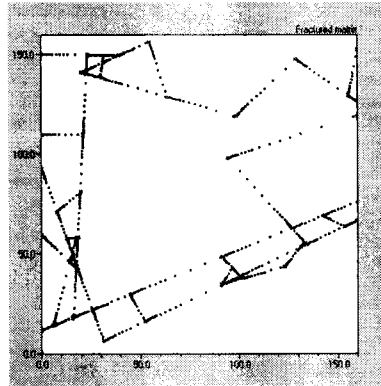


Figure 3. Example of transport nodes in a fractured medium ($\alpha_f=0.1$).

4. Conclusions

A new finite difference model is developed for solute transport in a fractured medium that can consider advection, adsorption, first-order decay, and scale-dependent dispersivity (α_f) of individual fractures. The scale-dependent α_f is simulated as a variable increasing with travel distance from a source using a numerical dispersion term caused by finite difference approximation. The developed model is free from numerical dispersion error, and is dependent only on the inlet concentration because the model simulates *artificially* a dispersion term in the convection-dispersion equation.

5. References

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