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Effect of Linear Sorption on Solute Transport in a Coupled Fracture-Matrix System with Sinusoidal Fracture Geometry

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Abstract: Modeling of solute transport through fractured rock is an important component of in many disciplines especially groundwater contamination and nuclear waste disposal. Several studies have been conducted on single rock fracture using parallel plate model and recently solute and thermal transport has been numerically modeled in the sinusoidal fracture matrix coupled system. The effect of linear sorption has been studied on the same. Results suggest the high matrix porosity and matrix diffusion coefficient enhance the sorption process and reduce the matrix diffusion of solutes. The velocity of the fluid reduces with increment in fracture aperture.

Key words: Sinusoidal fracture · Finite difference · Matrix diffusion · Linear sorption

INTRODUCTION

The behaviour of solutes has been studied widely in the past [1-4] and many others. In these studies, the processes such matrix diffusion [2, 5, 6] and sorption [6, 7] were identified as the dominant mechanisms affecting the solute mobility in the fractures. Thus, sorption along with matrix diffusion predominantly retards the solute movement. A common approach to the simulation of reactive solutes in fractured media is to assume that it is governed by a linear Freundlich sorption isotherm [2] and this has been widely used to model the transport of sorbing chemicals [8, 9]. The same has been considered for the present study.

The conceptual model for simulating solute transport in the coupled fracture matrix system is the dual porosity model considering the fractures to be parallel plates [2, 4, 10, 11, 12]. Significant research has been conducted in studying the adsorption of solutes in the fracture-matrix coupled system considering the fracture to be parallel plate model [13, 14, 15]. Many laboratory and field studies have observed that single fractures are not smooth parallel plates, but rather rough surfaces that are locally non parallel and potentially in contact [16, 17]. The sinusoidal fracture geometry provides the closest approximation of the real world fractures. Only a few studies have been conducted using sinusoidal fractures. Yeo [18] investigated the effect of fracture roughness on solute transport in a single fracture by assuming sinusoidal fracture geometry using Lattice Boltzmann method. Dijk and Berkowitz [19] examined the evolution of fracture aperture due to precipitation and dissolution in a sinusoidal fracture. Natarajan and Suresh Kumar [20, 21] have numerically simulated solute and heat transport in a coupled fracture matrix system with sinusoidal fracture geometry. Their model assumes an average velocity for the fracture but in this study velocity is assumed to vary with the fracture aperture. The aim of this paper is to study the effect of linear sorption of the solute transport mechanism in the coupled system with sinusoidal fracture geometry.

Physical System and Governing Equations: The conceptual model corresponding to sinusoidal fracture-matrix system is illustrated in Figure 1 below, where b refers to the varying half-fracture, H is the half fracture spacing, A is the amplitude of the sine wave, ë is the wavelength of the sine wave and L_f refers to the length of the fracture. The principal solute transport mechanisms in the fracture are advection, hydrodynamic dispersion and matrix diffusion and linear sorption. Solute migration in the fracture is considered to be faster than in the matrix and diffusion into the matrix is considered to be one dimensional process. Kennedy and Lennox [22] showed the validity of the assumption, that the diffusion exchanges along the direction perpendicular to the fracture are predominant, for most cases except for fractured clay with fracture aperture less than 20μm and flow velocities lower than 1m/day.

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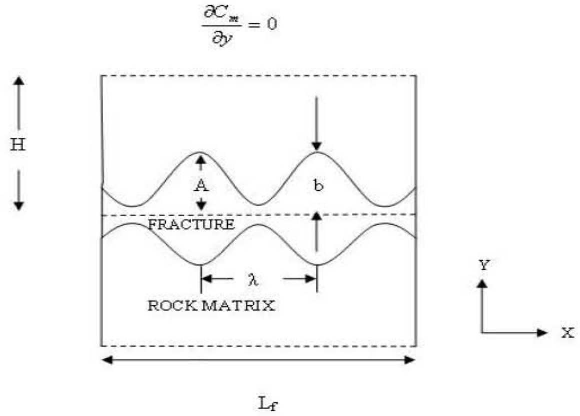

Fig. 1: Schematic representation of a fracture-matrix coupled system with sinusoidal fracture geometry with varying fracture aperture.

The transport equation was adopted for simulating solute transport along the fracture given by Tang *et al.* [2] has been modified to account for the varying fracture aperture.

$$R_f(x)\frac{\partial C}{\partial t} = D_L\frac{\partial^2 C}{\partial x^2} - V(x)\frac{\partial C}{\partial x} + \frac{\theta_m D_m}{b(x)}\frac{\partial C_m}{\partial y}\bigg|_{y=b} \tag{1}$$

Where

$$D_L(x) = \alpha V(x) + D_o \tag{2}$$

$$R_f(x) = 1 + \frac{K_f}{b(x)} \tag{3}$$

The equation for the impermeable rock-matrix is expressed as

$$R_m\frac{\partial C_m}{\partial t} = D_m\frac{\partial^2 C_m}{\partial y^2} \tag{4}$$

$$R_m = 1 + \frac{\rho_m K_m}{\theta_m} \tag{5}$$

Here R_f and R_m are retardation factors in the fracture and rock matrix [14], C_f and C_m are the volumetric concentrations of solute in high permeability fracture and low permeability rock-matrix respectively (ML^{-3}), x is the space coordinate along the flow direction in the fracture plane (L), y is the space coordinate perpendicular to the fracture plane(L), t is the time variable(T), b is the varying fracture aperture(L), V is the mean groundwater velocity in the fracture (LT^{-1}), θ_m is the matrix porosity, D_L is the hydrodynamic dispersion coefficient in the fracture (L^2T^{-1}), α is the longitudinal dispersivity in the fracture (L), D_o is the molecular diffusion coefficient of the solute in the water, D_m is the effective molecular diffusion coefficient in the rock-matrix, ρ_m is the bulk density of the rock matrix (ML^{-3}). The sorption coefficient K_f represents the partitioning between the amount of sorbed concentration of solute per unit fracture surface and the amount of aqueous concentration within the fracture (L) and similarly K_m represents the adsorptive loss of solute within the solid rock matrix (L^3M^{-1}). This refers to the partitioning between the sorbed concentration of solute per unit volume and the amount of aqueous concentration. The sorption coefficients cause retardation of the solute in the fracture and the rock-matrix. Expressions (3) and (5) are valid for instantaneous linear equilibrium sorption isotherms.

The term on the left hand side of Eqn. (1) represents change of solute mass in the fracture and on the right hand side the first term represents the dispersive flux, the second term represents the advective flux and the last term represents the mass transfer term fracture to matrix. Eqn. (4) represents solute transport in impermeable rock-matrix by diffusion. The initial and boundary conditions associated with Eqn. (1) and Eqn.(4) are

$$C_f(x, t = 0) = 0 \tag{6}$$

$$C_m(x, y, t = 0) = 0 \tag{7}$$

$$C_f(x = 0, t) = C_o \tag{8}$$

$$C_f(x = L_f, t) = 0 \tag{9}$$

$$C_m(x, y = b, t) = C_f(x, t) \tag{10}$$

$$\frac{\partial C_m}{\partial y}\bigg|_{(x, y = H, t)} = 0 \tag{11}$$

And for $b \le y \le H$,

$$\frac{\partial C_m}{\partial x}\bigg|_{(x = 0, t)} = 0 \tag{12}$$

$$\frac{\partial C_m}{\partial y}\bigg|_{(x = L_f, t)} = 0 \tag{13}$$

Where C_o is the injected concentration at the inlet of the fracture (ML^{-3}).

Numerical Model: The system is described by a set of coupled partial differential equations, one for the fracture and another for the matrix, formulated in pseudo two dimensional framework. The set of partial differential equations are solved numerically. Among the various numerical schemes such as finite element, finite difference and finite volume, a finite difference scheme has been adopted for developing this model. A fully implicit finite difference scheme is used to obtain a closer approximation and moreover implicit scheme provides more accurate results compared to the explicit scheme. The model developed is used for understanding the effect of sorption on the solute transport in the coupled system with sinusoidal fracture. To satisfy the continuity at the fracture matrix interface, iteration is performed at each time step. A varying grid is adopted at the fracture matrix interface to accurately capture the flux at the interface. A wavelength of 4m and amplitude of 66μm was adopted for simulating the sinusoidal wave, using which the varying aperture values were generated for the numerical model. A fracture length of 50m and a simulation period of 10 days were adopted for the simulation.

RESULTS AND DISCUSSION

A numerical model has been developed to study the effect of linear sorption in the fracture-matrix coupled system with sinusoidal fracture geometry. The parameters used for the simulation has been tabulated below.

The numerical model was validated with the analytical solution provided by Sudicky and Frind [23] for solute transport with linear sorption using the parallel plate model.

Figure 2 shows the validation of the numerical model with the analytical solution provided by Sudicky and Frind [23] for solute transport undergoing linear sorption in a coupled fracture matrix system using the parallel plate model. It is observed from Figure 2 that the numerical results are in close agreement with the analytical solution which illustrates the robustness of the numerical model.

Figure 3 provides the spatial distribution of relative concentration for different matrix diffusion coefficients obtained using the sinusoidal fracture geometry. It is observed from Figure 3 that when the matrix diffusion coefficient is very high, the solutes sorbed on the sinusoidal fracture wall surface hinder the diffusion of solutes into the rock matrix and further the solutes get stagnated in the curvature. As a result of which the relative concentration of solutes in the fracture is very high in the inlet of the fracture. On the other hand, when the diffusion coefficient is very low, solute concentration reaches zero very

Table 1: Parameters used for the numerical simulation

Parameter	Symbol	Value	Unit
Initial fracture aperture	2b	200	μm
Fluid velocity	V	1	m/day
Dispersivity	α	0.05	m
Matrix porosity	θ_m	0.05	
Hydrodynamic dispersion coefficient	D	1e-06	m^2/d
Initial concentration at the inlet of the fracture	C_O	1	
Partitioning coefficient within the fracture	K_f	1e-04	m
Partitioning coefficient within the rock-matrix	K_m	7.5e-04	m^3/kg
Bulk density of the rock matrix	ρ_m	2000	kg/m^3
Half fracture spacing	H	0.1	m
Length of the fracture	L	50	m
Total simulation time	T	10	day

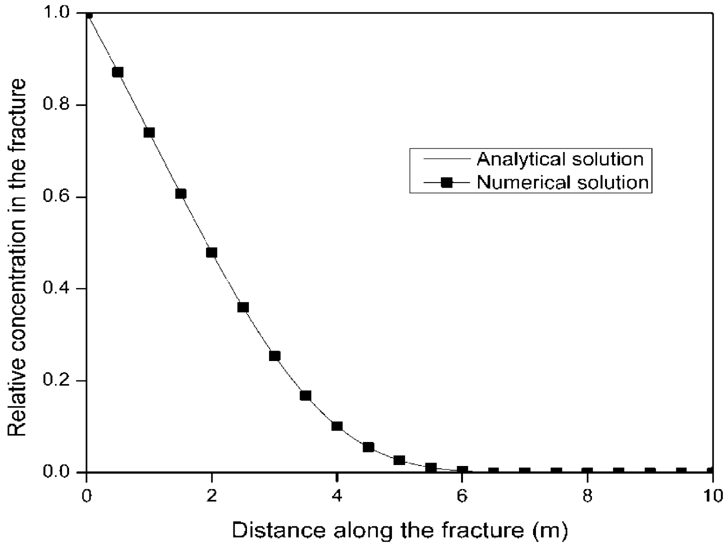

Fig. 2: Validation of numerical results obtained using the parallel plate model with analytical solution (Refer Table 1 for data)

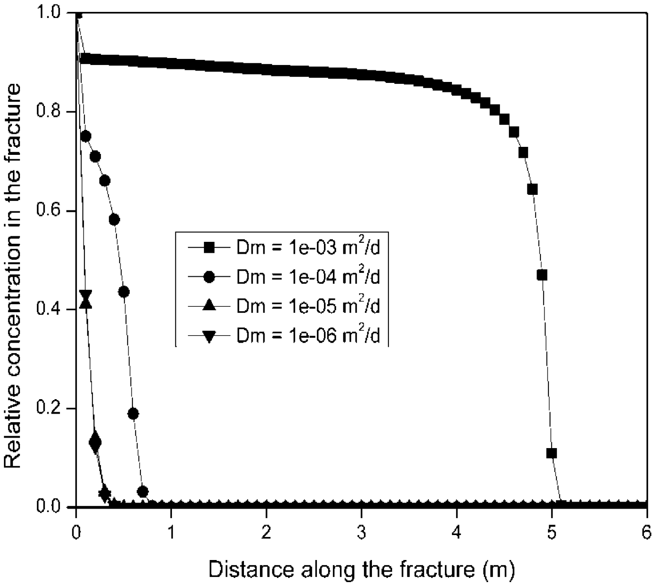

Fig. 3: Spatial distribution of relative concentration for different matrix diffusion coefficients obtained using sinusoidal fracture geometry (Refer to table 1 for other data)

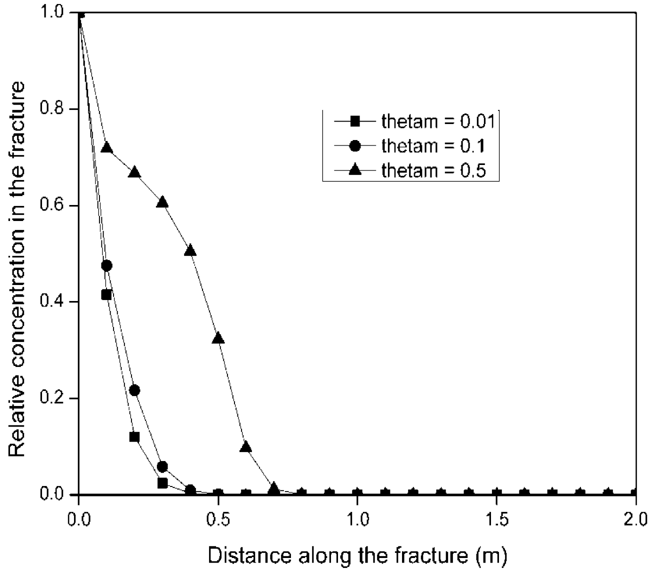

Fig. 4: Spatial distribution of relative concentration for different matrix porosity obtained using sinusoidal fracture geometry (Refer to table 1 for other data)

close to the fracture inlet as there is less sorption of solutes on the fracture walls and consequently matrix diffusion is relatively high.

Figure 3 provides the spatial distribution of relative concentration for different matrix porosity values obtained using the sinusoidal fracture geometry. Generally, high matrix porosity enhances matrix diffusion and subsequently the solute concentration would reach zero quickly in the fracture but here a reverse behavior is observed. This is because the solutes adsorbed on the curvatures of the sinusoidal fracture is high when the matrix porosity is high, resulting from high partitioning coefficient. This causes low matrix diffusion. On the other hand, sorbed concentration is lower when the matrix porosity is low, resulting in high diffusion of solutes.

Figure 5 provides the spatial distribution of the fluid velocity in the sinusoidal fracture. It is observed from Figure 5 that the velocity of the fluid is high when the half

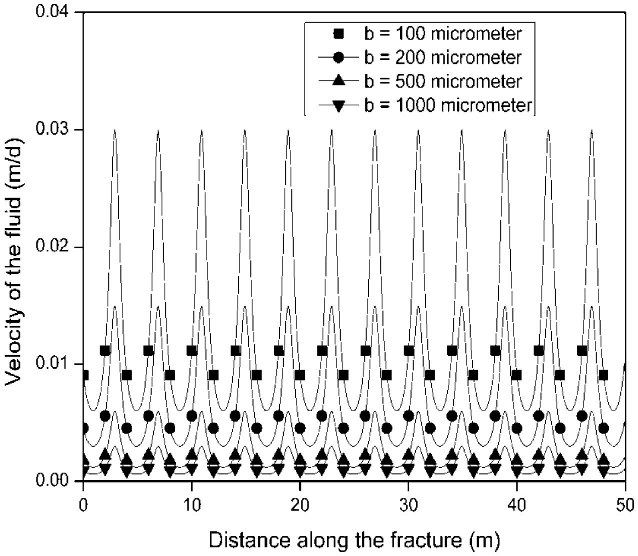

Fig. 5: Spatial distribution of velocity of the fluid obtained using sinusoidal fracture geometry (Refer to table 1 for other data)

fracture aperture is very small. As the half fracture aperture is increased, the velocity of the fluid reduces along the fracture. It is also observed the pattern adopted by the velocity profile is similar to the sinusoidal fracture geometry. The velocity of the fluid is high at the ridges and it is low at the troughs. The fracture aperture values adopted here are considered as averaged values.

CONCLUSION

The effect of linear sorption on solute transport in sinusoidal fracture matrix coupled system has been attempted. A high matrix porosity and diffusion coefficient enhances the sorption of solutes as the partitioning coefficient is increased. This results in higher solute concentration in the fracture. The amount of mass diffused into the rock-matrix varies spatially along the fracture due to the sinusoidal nature of the fracture. The velocity of the fluid reduces as the average fracture aperture is increased.

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