Numerical modeling of solute transport in a coupled sinusoidal fracture matrix system in the presence of fracture skin

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Abstract— Modeling of fluid flow and solute transport through fractured rock is an important aspect of many disciplines such as groundwater contamination, nuclear waste disposal, petroleum and gas production, mine excavation and geothermal production. A few studies have been conducted in the coupled fracture matrix system in the presence of fracture skin using parallel plate model. An attempt has been made to simulate solute transport in sinusoidal fracture-skin-matrix coupled system numerically. Results suggest that the spatial variation of the fracture aperture along the fracture affects the mass transfer at the fracture-skin interface. The sinusoidal fracture geometry increases the residence time of the solutes and thus increases the rate of diffusion of solutes into the fracture skin. The sinusoidal geometry of the fracture plays a major role in the mass transfer mechanism and thus needs to be considered while modeling contaminant transport in the fractures.

***Keywords*—** Sinusoidal fracture, Fracture skin, Finite difference, matrix diffusion.

I. INTRODUCTION

Fractures in geological formations are of interest for many researchers around the globe as they play a major role in many disciplines such as reservoir exploration for water supply, contamination of subsurface repositories, petroleum extraction from the subsurface, geothermal energy production and so on. Substantial research has been conducted on solute transport in a coupled fracture matrix system (Grisak and Pickens 1980; Tang et al. 1981; Maloszewski and Zuber 1985, 1990, 1992;Wallach and Parlange 1998; Cvetkovic et al. 1999; Tsang and Tsang 2001; Sekhar et al. 2006; Sekhar and Suresh Kumar 2006; Suresh Kumar 2008). Recent studies have revealed the presence of a small portion just adjacent to the rock matrix with properties quite different to that of the rock matrix. This portion is called as the fracture skin. These are defined as low-permeability material deposited along the fracture walls. Sharp (1993) pointed out the possibility of the presence of fracture-skins in a fractured porous media. A few studies conducted with respect to solute transport in fracture-skins have concluded that fracture-skins in the form of clay filling (Driese et al. 2001), mineral precipitation (Fu et al. 1994) and organic growth material (Robinson and Sharp 1997) have reduced the permeability in fracture-skin while some others have concluded that the presence of fracture-skins has increased the permeability in fracture-skins by developing micro-fractures (Polak et al. 2003). Since the properties of the fracture skin are different from that of the rock matrix, transport through the fracture skin can significantly affect the transport mechanism in the system. Robinson et al. (1998) provided an analytical solution for the contaminant transport in a set of parallel fractures with fracture skin. Zimmerman et al. (2002) studied the effect of sorption of solutes on the altered fracture surfaces using an experimental procedure. Garner and Sharp (2004) analyzed the solute transport in granitic rocks with fracture skin using the data from two different field sites. It is observed that a few studies have been conducted in the coupled fracture matrix system in the presence of fracture skin and the above models have been developed using the traditional parallel plate model. As far as the knowledge of the authors' concerned, no studies have been conducted in the fracture skin matrix system with sinusoidal fracture geometry. Although the transport mechanism in the fracture matrix coupled system is modeled using the parallel plate model, it is a well known fact that in reality fractures are not parallel plates. Many laboratory and field studies have observed that the fractures are rough surfaces that are locally non plannar and non parallel (Hakami and Barton 1990, Brown 1995). The geometry of the fracture does play a major role on the transport mechanism. Some researchers have considered the fractures to possess sinusoidal geometry. Dijk and Berkowitz (1998) examined the evolution of fracture aperture in sinusoidal fracture geometry due to precipitation and dissolution. Yeo (2001) investigated the effect of fracture roughness on solute transport in a single fracture by assuming sinusoidal fracture geometry using Lattice Boltzmann method.

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Natarajan and Suresh Kumar(2010 a,b) have numerically modeled solute transport and thermal transport in a coupled fracture matrix system with sinusoidal fracture geometry. The objective of the present study is to analyse the solute transport mechanism in the sinusoidal fracture matrix system in the presence of fracture skin. As the fracture aperture is spatially varying along the fracture length, a varying velocity is considered for this model.

II. PHYSICAL SYSTEM AND GOVERNING EQUATIONS

The conceptual model corresponding to a coupled fracture-skin-matrix system (Robinson et al. 1998) is illustrated in Fig.1. below, where b refers to the varying half-fracture, H is the half fracture spacing, A is the amplitude of the sine wave, δ 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. 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 (2005) 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.

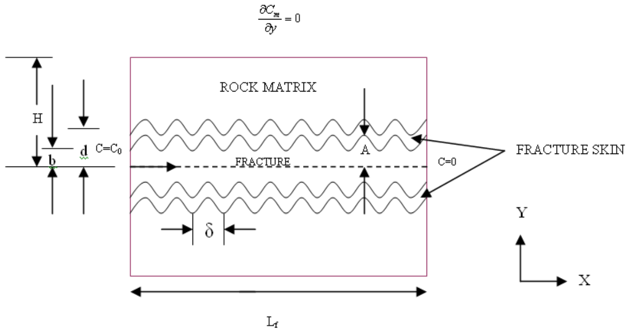

Fig. 1 Schematic diagram showing a coupled sinusoidal fracture-skin-matrix system

The governing equations for modeling solute transport in the coupled fracture skin matrix system provided by Robinson et al.(1998) has been modified for the present problem.

$$R_f(x)\frac{\partial C_f}{\partial t} = D_L\frac{\partial^2 C_f}{\partial x^2} - V_0\frac{\partial C_f}{\partial x} - \lambda C_f + \frac{\theta_s D_s}{b}\frac{\partial C_s}{\partial y}\Big|_{y=b} \quad (1)$$

Where

$$D_L(x) = \alpha V(x) + D_o$$

(2)

The equations for low-permeability fracture-skin and rock-matrix are expressed as

$$R_s\frac{\partial C_s}{\partial t} = D_s\frac{\partial^2 C_s}{\partial y^2} - \lambda C_s$$

(3)

$$R_m\frac{\partial C_m}{\partial t} = D_m\frac{\partial^2 C_m}{\partial y^2} - \lambda C_m$$

(4)

Here C_f, C_s and C_m are the volume concentrations of solute in high permeability fracture, low permeability fracture-skin 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 coordinate (T), D_L is the hydrodynamic dispersion coefficient in the fracture (L^2T^{-1}), α_0 is the longitudinal dispersivity in the fracture (L), D_0 is the molecular diffusion coefficient of solute in free water (L^2T^{-1}), D_s and D_m are effective diffusion coefficients in fracture-skin and rock-matrix respectively, λ is first order radio-active decay constant (T^{-1}). R_f, R_s and R_m are the retardation factors in fracture, fracture-skin and rock-matrix respectively and are expressed as

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

(5)

$$R_s = 1 + \frac{\rho_s K_s}{\theta_s}$$

(6)

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

(7)

In Eqn (5), K_f is the surface sorption coefficient of fracture (L), which represents the effect of adsorption of solute on the fracture walls. This sorption on the fracture walls represents the partitioning between the amounts of sorbed concentration of solute per unit surface and finally results in a retardation of solute with respect to mobile fluid within the fracture. K_s represent the adsorptive loss of solute within the fracture skin. This sorption within the low permeability fracture-skin represents the partitioning between the amount of sorbed concentration of solute per unit volume and amount of aqueous concentration and eventually causes retardation of solute with respect to immobile fluid within the fracture-skin. Similarly K_m represents the adsorptive loss of solute within the porous rock-matrix. Expressions (5), (6) and (7) are valid for instantaneous linear equilibrium sorption isotherms.

It is assumed that there is no solute in the system at the beginning of numerical simulation and the upstream end in the fracture is subjected to a constant source boundary condition of Dirichlet type. A zero flux boundary condition (Neumann type) is commonly employed at the end of the fracture. However in the present study the downstream boundary is assumed to be far away such that the concentration front does not reach this location during the simulation period, and hence, a Dirichlet type boundary condition of zero concentration at the outlet is adopted.

The initial and boundary conditions associated with equations (1), (3) and (4) are:

$$C_f(x,\ t=0)=C_s(x,\ y,\ t=0)=C_m(x,\ y,\ t=0)=0$$

$$C_f(x=L_f,\ t)=0$$

(10)

$$C_f(x,\ t)=C_s(x,\ y=b,\ t)$$

(11)

$$\theta_s D_s\frac{\partial C_s(x,\ y=d,\ t)}{\partial y}=\theta_m D_m\frac{\partial C_m(x,\ y=d,\ t)}{\partial y}$$

(12)

$$C_s(x,\ y=d,\ t)=C_m(x,\ y=d,\ t)$$

(13)

$$\frac{\partial C_m(x,\ y=H,\ t)}{\partial y}=0$$

(14)

The following assumptions have been made while developing this model:

1. Advection is considered to be negligible in rock-matrix as well as fracture skin.
2. Transverse diffusion and dispersion within the fracture assures complete mixing across fracture width at all times.
3. Width of fracture is assumed to be much smaller than the length of the fracture.
4. Permeability of rock matrix is low, and molecular diffusion is assumed to be the main transport mechanism in rock-matrix and fracture skin.
5. Transport in the fracture is considered to be much faster than transport in rock-matrix.
6. Fracture, fracture skin and rock matrix is assumed to be fully saturated.
7. Reversible sorption within the fracture, fracture-skin and rock-matrix is accounted for by a retardation factor.
8. It is assumed that reactions taking place between (i) fracture and fracture-skin, and (ii) fracture-skin and rock-matrix are instantaneous, i.e., an equilibrium between the solute in the fluid and the adsorbed mass is very rapid compared to the characteristic time of transport.
9. The solution is restricted to an elementary part of the system, for example, one half of a high permeability fracture, its adjacent low permeability fracture-skin and its associated one half of rock-matrix by assuming symmetry.

III. NUMERICAL MODEL

In this study, the system is described by a set of three partial differential equations, containing one equation for the fracture, one for fracture-skin and the rest for the rock-matrix, formulated in a one-dimensional framework. Second-order central difference finite difference scheme is used to solve this system numerically. Solution is iterated at each time step in order to satisfy the continuity at the high and low permeability interface, i.e., fracture-skin interface. Uniform grid size is adopted in the fracture whereas a non-uniform grid size is adopted along fracture-skin as well as rock-matrix. A smaller grid size is adopted at the fracture-skin interface to accurately simulate the concentration flux at the fracture-skin interface.

(8) $C_f(x=0,\ t)=C_0$

The discritization of the coupling term representing the last term on the right hand side of Eq. (1), involves the difference in the fracture/skin concentrations over the fracture-skin interface between the second and first nodes of fracture-skin. Thus the coupling term in Eq. (1) is discretized as

$$\frac{\partial C_s}{\partial y}=\frac{C_{s\ 2}^{n+1}-C_{s\ 1}^{n+1}}{\Delta y_s(1)}$$

(15)

Where Δy_s (1) represents the cell width across the fracture-skin interface.

Here the concentration at the first node in the fracture-skin, i.e., $C_{s\ 1}^{n+1}$, will be equal to the corresponding fracture concentration $\left(C_{f\ i}^{n+1}\Big|_{i=1}\right)$ perpendicular to the fracture-skin satisfying assumed boundary condition, that is,

$$C_{s\ 1}^{n+1}=C_{f\ 1}^{n+1}$$

(16)

The concentration of the second node in the fracture-skin, $C_{s\ 2}^{n+1}$, at unknown at the next time level, (n+1)th time level, it will become fourth unknown. The value of this unknown is assumed and iterated till convergence. Thus using Tridiagonal

Thomas algorithm (TTA), the three unknowns that are solved for the fracture are at Ith node, (I-1)th node and (I+1)th node, at (n+1)th time level. Thus, the fourth unknown, the concentration at the second node of the skin at (n+1)th level, $C_{s\ 2}^{n+1}$ is not solved by TTA solver as its value is assumed at (n+1)th level and iterated until convergence.

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.

Parameters	Values
Fracture dispersivity (α_o)	0.001 m
Longitudinal Dispersion coefficient within the fracture (D_L)	1x10^{-3} m^2/d
Free molecular diffusion coefficient in water (D_0)	1x10^{-6} m^2/d
Effective diffusion coefficient in the rock matrix (Dm)	4x10^{-6} m^2/d
Effective diffusion coefficient in the fracture-skin (Ds)	4x10^{-7} m^2/d
Porosity of rock-matrix (θm)	0.145
Porosity of fracture-skin (θs)	0.035
Length of fracture (L_f)	50 m
Fracture spacing (2H)	0.31 m
Half fracture aperture (b)	0.0001 m
Fracture-skin thickness (d-b)	0.002 m
Total simulation time	10 days
Coefficient of radioactive decay(λ)	6.33x10^{-5} d^{-1}

IV. RESULTS AND DISCUSSION

A numerical model has been developed to analyze solute transport in a coupled fracture-matrix coupled system with sinusoidal fracture geometry in the presence of fracture skin. The parameters used for the simulation has been tabulated below.

Table I Parameters used for the numerical simulation

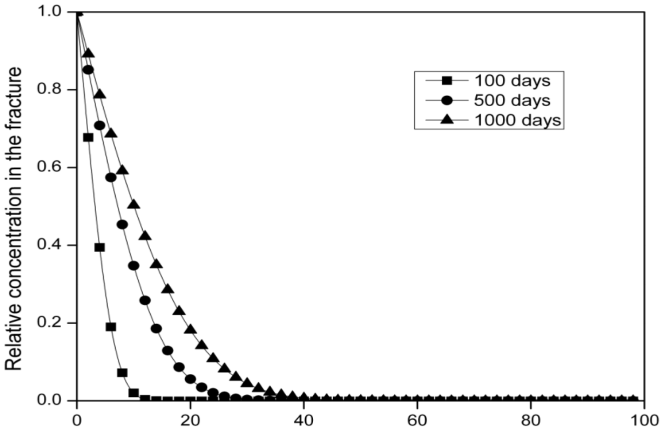

Fig. 2 Validation of numerical results with analytical solution provided by Robinson et al. (1998) (Average velocity of the fluid = 1 m/d, Dispersion coefficient of fracture = 10^{-3}m^2/d, Diffusion coefficient in the rock matrix = 4x10^{-6}m^2/d, Diffusion coefficient in the fracture skin = 4x10^{-7}m^2/d, Porosity of the rock matrix = 0.145, Porosity of the fracture skin = 0.0145, Length of the fracture = 100m, Half fracture aperture = 0.0002m,

The results for the verification of the numerical model for solute transport in a fracture skin matrix system with parallel plate model have been shown in Fig. 2. The analytical solution of Robinson et al. (1998) has been represented by solid lines, while the numerical results have been plotted in terms of data points. The results confirm that the numerical model follows a close agreement with the results of the analytical solution and thus ensures the robustness of the numerical model.

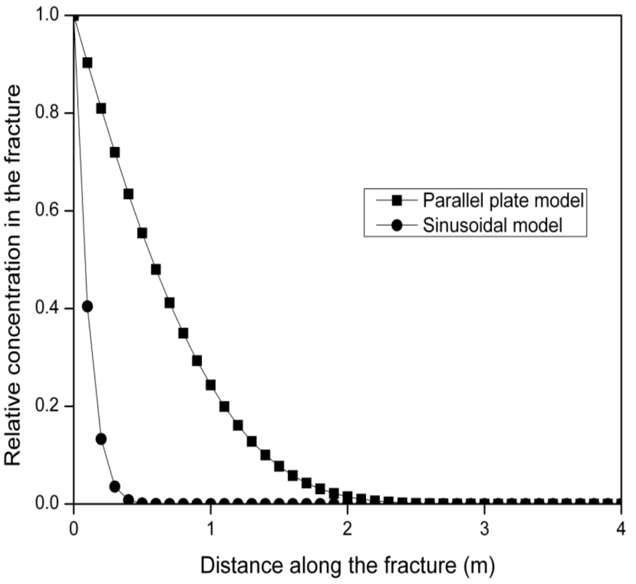

Fig.3 Comparison of relative concentration of solutes obtained from the parallel plate model and sinusoidal model (R_s = 673, R_m = 141, Refer to table 1 for other data).

Fig.3 provides the comparison of the relative concentration of solutes obtained using parallel plate and sinusoidal model. It is observed from Figure 3 that the concentration obtained using the sinusoidal model reaches zero concentration very near to the fracture inlet compared to the parallel plate model due to sinusoidal curvature of the fracture aperture. Thus, the geometry of the aperture plays an important role in solute transport mechanism in the fracture matrix skin system.

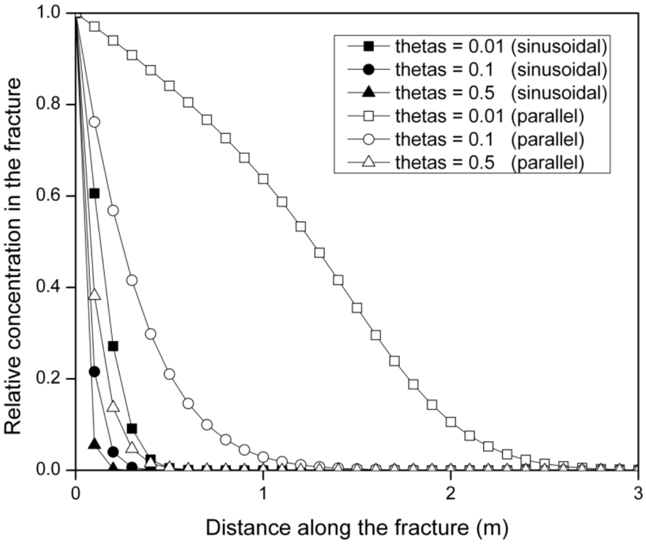

Fig. 4 Comparison of relative concentration obtained from parallel plate and sinusoidal models for different skin porosities (R_s = 673, R_m = 141, Refer to table 1 for other data).

Fig. 4 illustrates the comparison of spatial distribution of relative concentration of solutes for various skin porosities obtained from the parallel plate model and the sinusoidal model. It is observed from Figure 4 that there is a huge difference between the concentration profiles obtained from both the models for the same porosity value. As the porosity of the skin is increased from 0.01 to 0.5, the concentration in the fracture reduces in both the models. When the skin porosity is low, the sinusoidal model behaves similar to the parallel plate model. With increment in porosity, the concentration in the sinusoidal fracture still remains low as the curvature of the fracture increases the rate of diffusion of solutes from the fracture into the skin. Thus, the mass transfer mechanism in the sinusoidal model varies from that of the parallel plate model.

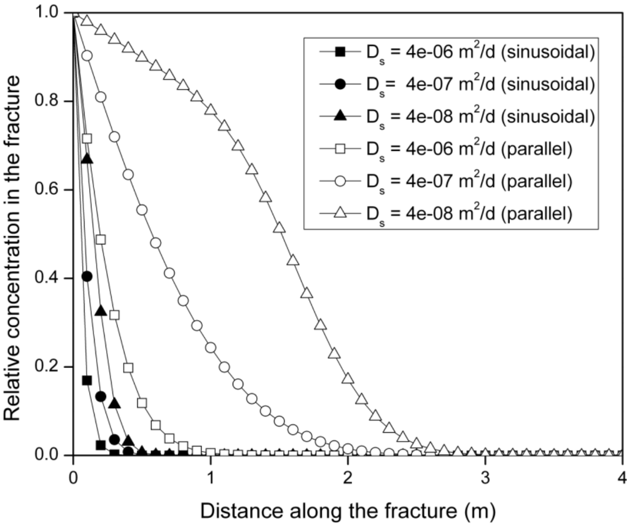

Fig. 5 Comparison of relative concentration obtained from parallel plate and sinusoidal models for different skin diffusion coefficients (R_s = 673, R_m = 141, Refer to table 1 for other data).

Fig. 5 illustrates the comparison of spatial distribution of relative concentration of solutes for various skin porosities obtained from the parallel plate model and the sinusoidal model. It is observed from Figure 4 that as the diffusion coefficient of the skin is increased from 4e-08 to 4e-06 m^2/d, the concentration in the fracture reduces in both the models but in the sinusoidal model the variation is very low and the concentration reaches zero within 1m from the fracture inlet. With increment in diffusion coefficient, the concentration in the sinusoidal fracture remains low as the curvature of the fracture increases the residence time of the solutes in the fracture which enhances the diffusion of solutes into the fracture skin.

V. CONCLUSION

Numerical modeling of solute transport in a coupled sinusoidal fracture matrix system in the presence of fracture skin has been attempted. The sinusoidal model behaves differently from the parallel plate model in the presence of fracture skin. The sinusoidal curvature provides high residence time for the solutes and thus enhances the diffusion of solutes into the fracture skin. Thus, the geometry of the fracture has a significant impact on the mass transfer mechanism in the fracture skin matrix system.

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