Colloidal transport in a coupled sinusoidal fracture matrix system

N.Natarajan[1*] and G. Suresh Kumar[2]

Abstract— Colloids act as carriers of contaminants in the subsurface media and thus modeling of colloidal transport through fractures has gained importance in the recent decades. Several studies have been conducted on colloid transport in rock fractures using the traditional parallel plate model while only a few have addressed the same in irregular fractures with varying apertures. An attempt has been made to simulate colloidal transport in sinusoidal fracture-matrix coupled system numerically. Results suggest that the sinusoidal fracture model behaves differently from the parallel plate model as the fracture aperture in the sinusoidal fracture is varying spatially along the fracture as well as within the same cross section of the fracture. Filtration and remobilization of colloids has negligible effect on the colloidal concentration in the sinusoidal fracture matrix system. For high diffusion coefficients of the colloids, the concentration of colloids in the fracture is very significant which is different from the usual behaviour resulting from the geometry of the fracture aperture and the proportion of colloids diffusing into the rock matrix

Keywords— Colloidal transport, sinusoidal fracture, finite difference, rock matrix, remobilisation

I. INTRODUCTION

Colloidal transport in fractured media is very important phenomenon because of the potential of the colloids in facilitating the movement of radionuclides in the subsurface media. Colloids have been observed in the transport of contaminants in many studies (Champ et al. 1984, Eichholz et al. 1982, Kretzschmar et al. 1999, Penrose et al. 1990, Buddemeier and Hunt 1998, Walton and Merritt 1980, McCarthy et al. 1998a,b, Short et al. 1998, Kersting et al. 1999). The sorption of contaminants on colloids can affect the transport mechanism of the contaminants in fractured media as

[1]Research Scholar, EWRE Division, Department of Civil Engineering, Indian Institute of Technology, Madras, Chennai-36, India. E-mail: itsrajan2002@yahoo.co.in
[2]Associate Professor, Department of Ocean Engineering, Indian Institute of Technology, Madras, Chennai – 36, India. E-mail: gskumar@iitm.ac.in

the sorbed contaminants are not subjected to retardation mechanisms like matrix diffusion and thus enhancing the mobility of the contaminants (Baek and Pitt 1996). Thus analysis of colloids is very important as they act as carriers for the contaminants and thus influence their rate of migration.

Colloids are tiny particles in the size range of 1 nm to 1μm suspended in water, with high surface area and electrostatic charge (Hunter 1986). The natural colloids in groundwater and the repository derived colloids influence the radionuclide migration significantly since they are smaller than the intergranular pores and fractures in rock and have the capacity to travel long distances in percolating waters (Li et al. 2004). Colloids are present in the subsurface in the form of bacteria, viruses, metal oxides, clay minerals and humic macromolecules (Mills et al. 1991, Moulin and Ouzounian 1992).

Many researchers have developed models for colloidal transport in the subsurface media. Hwang et al. (1990) presented a model for colloid migration in a single planar fracture with the assumption that colloids are not depositing on fracture surfaces. Champ et al. (1984) observed rapid transport of bacterial colloids relative to conservative tracers in a field experiment in crystalline fractured rocks. Abdel-Salam and Chrysikopoulos (1994) presented analytical solution to the problem of colloid transport in a single fracture for constant concentration as well as constant flux boundary conditions. McCarthy and McKay (2004) described the challenges in the analysis of colloid transport in natural settings. James and Chrysikopoulos (2003) derived analytical solutions for monodisperse and polydisperse colloid transport in uniform fractures. Substantial studies have been conducted on colloid transport considering the fractures to be smooth, parallel plates. Only a few studies have accounted for the aperture variation spatially.

Chrysikopoulos and Abdel-Salam (1997) developed a numerical model to describe the transport of colloids in a saturated fracture with spatially variable aperture, accounting for colloid deposition onto fracture surfaces under various physicochemical conditions using stochastic modeling. James et al. (2005) presented a quasi-three dimensional particle

tracking model to analyze the transport of contaminants in the presence of colloids through a variable fracture aperture situated in the porous medium. A probabilistic form of the Boltzmann law was used to describe filtration of both colloids and contaminants on fracture walls. Their study has not included the effect of remobilization of colloids. Earlier studies have shown that the changes in the subsurface conditions, such as pH and ionic strength, can remobilize previously filtered colloids (Vilks et al. 1996, McCarthy and Degueldre 1993). Thus remobilization of colloids is one of the important parameter which needs to be taken into account while modeling colloidal transport. Remobilization process has been considered while modeling colloidal transport (Anghel and Reimus 2000, Reimus et al. 2003). Apart from the parallel plate model, a few researchers have carried out studies on sinusoidal and saw toothed fractures.

Zimmerman et al. (1991) studied the permeability of rough fractures using the lubrication theory. They applied the lubrication theory to two simplified aperture profiles, sinusoidal as well as saw tooth and derived analytical expressions for the permeabilities. 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. Recently, Natarajan and Suresh Kumar (2010a,b) have simulated solute transport and thermal transport in a coupled sinusoidal fracture matrix system numerically. However, colloidal transport differs from contaminant transport (Keller and Auset 2004). None of the previous studies have attempted to analyse the transport of colloids in a sinusoidal fracture. The objective of the present study is to investigate the effect of various colloidal transport properties on the evolution of colloidal concentration in a coupled sinusoidal fracture matrix system. Filtration as well as remobilization of colloids has been incorporated into the present model.

II. 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, δ is the wavelength of the sine wave and L_f refers to the length of the fracture. The principal colloidal transport mechanisms in the fracture are advection, hydrodynamic dispersion and matrix diffusion. Colloidal 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.
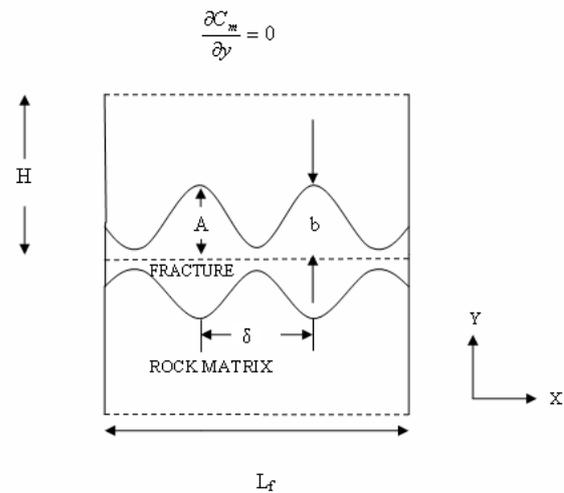
Figure 1. Schematic representation of a fracture-matrix coupled system with sinusoidal fracture geometry with varying fracture aperture.

The transport equation was adopted for simulating colloidal transport along the fracture given by Li et al. (2004) has been modified to account for the varying fracture aperture.

$$\frac{\partial}{\partial t}\left(C + \frac{\sigma_C}{b(x)}\right) + V_C(x)\frac{\partial C}{\partial x} - D_C\frac{\partial^2 C}{\partial x^2} + \frac{Q_C}{b(x)} = 0$$
(1)

$$\frac{\partial \sigma_C}{\partial t} = \lambda_f V_C C b(x) - Rmb\sigma_c$$
(2)

Q_C is the diffusion flux of the colloids from the fracture into the rock-matrix and

$$Q_C = -\varepsilon\theta\frac{\partial C_P}{\partial z}\bigg|_{z=b}$$
(3)

ε is the percentage of matrix flux diffusion into the rock-matrix since the diffusion of colloids may be hindered by the colloids filtered on the fracture surface and some colloids with diameters larger than the pores in the rock-matrix cannot diffuse into the rock-matrix.

The governing equation for the colloid transport in the rock matrix is expressed as:

$$(1 + K_{d_{CP}})\frac{\partial C_P}{\partial t} - D_{CP}\frac{\partial^2 C_P}{\partial z^2} = 0$$
(4)
$$x > 0, z \geq b, t \geq 0$$

Where C_P is the concentration of the colloids in the porous rock matrix, D_{CP} is the diffusion coefficient of the colloids and $K_{d_{CP}}$ is the sorption partition coefficient for the colloids within the rock matrix.

The initial and boundary conditions for colloid transport are given as:

$C(x = 0, t) = C_0$ (5)

$C(x = L, t) = 0$ (6)

$C(x, t = 0) = C_P(x, z, t = 0) = 0$ (7)

$C_P(x, z = b, t) = C(x, t)$ (8)

$$\frac{\partial C_P(x, z = H, t)}{\partial z} = 0$$ (9)

Where C_o is the concentration of the colloids at fracture inlet

III. 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 equations are solved numerically using fully implicit finite difference scheme. 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 years were adopted for the simulation. A constant discharge of $5 \times 10^{-5} m^3/d$ and a varying velocity has been assumed for the present study.

IV. RESULTS AND DISCUSSION

A numerical model is developed to simulate colloidal transport in a coupled sinusoidal fracture matrix system. The numerical model using the conventional parallel plate fracture system was validated with the analytical solution provided by Van Genuchten (1981). The base case data pertaining to colloids was adopted from Abdel-Salam and Chrysikopolous (1994). The parameters used for validation of the numerical results with the analytical solution for colloids are presented in Table1. The results for the verification of the model have been shown in Figure. 2.

Table I Parameters used for the numerical simulation

Parameter	Symbol	Value
Initial half-fracture aperture (m)	b	1.25e-04

| Parameter	Symbol	Value
Fluid velocity (m/year)	V	1
Hydrodynamic dispersion coefficient in the fracture (m²/year)	D	0.25
Length of the fracture (m)	L_f	150
Total simulation time (day)	T	5
Colloid dispersion coefficient (m)	κ	1e-10
Concentration of colloids at the inlet of the fracture (kg/m³)	C_o	1
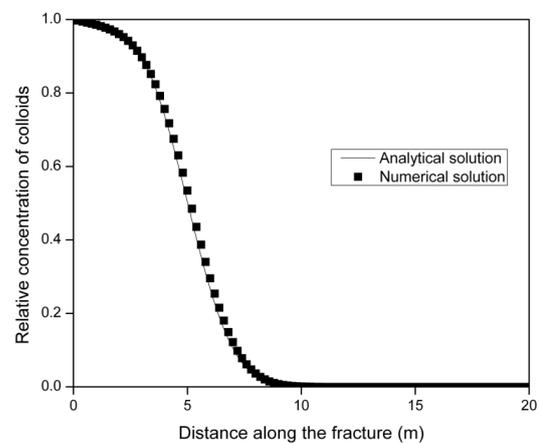
Figure 2. Validation of numerical results with analytical solution for colloid transport in a single rock fracture. Refer to Table 1 for data.

The analytical solution is represented by solid lines while the numerical solution is represented by data points. It is observed from Figure. 2 that the numerical results are in close agreement with the analytical solution for the data provided in Table 1, which illustrates the robustness of the numerical model. The parameters used for numerical simulation of colloid transport in the sinusoidal fracture matrix system are provided in Table 2.

Table 2. Parameters used for the colloid transport in sinusoidal fracture matrix system

| Parameter	Symbol	Value
Initial half-fracture aperture (m)	b	100e-06
Fracture spacing (m)	2H	0.1
Porosity of the rock matrix	θ	0.09

Colloid concentration at the inlet of the fracture (kg/m^3)	C_o	1
Hydrodynamic dispersion coefficient of colloids suspended in the rock fracture (m^2/year)	D_C	1
Filtration coefficient for colloids (m^{-1})	λ	0.5
Percentage of diffusion for colloids	ε	0.5
Diffusion coefficient of colloids within the fracture-skin (m^2/year)	D_{CP}	2.2e-08
Distribution coefficient for colloids within the rock-matrix	$K_{d_{CP}}$	0.1
Remobilisation coefficient for colloids in the fracture (year^{-1})	Rmb	0.5
Length of the fracture (m)	L	50
Total simulation time (year)	T	10
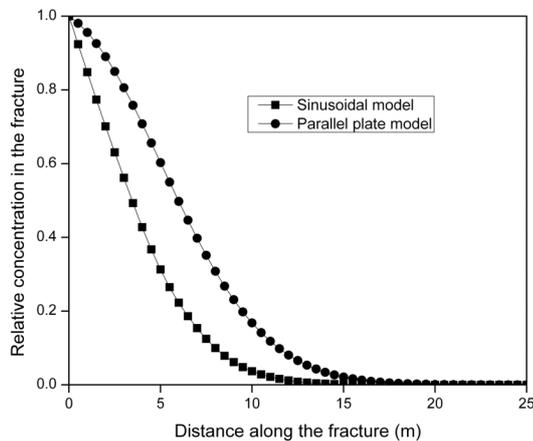
Figure 3. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models. Refer Table 2 for base case parameters.
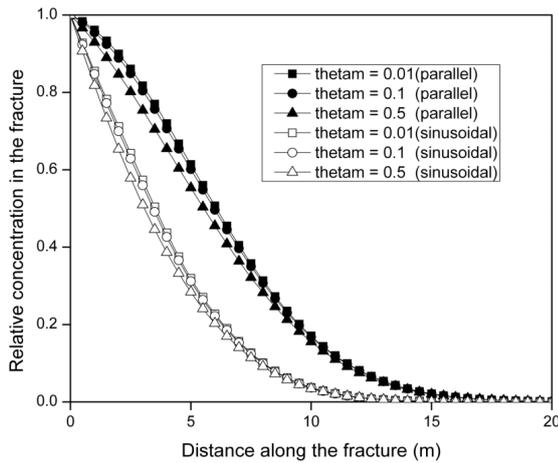
Figure 3 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal fracture model. It is observed from Figure 3 that the relative concentration of colloids from the parallel plate model reaches zero concentration at 20m from the fracture inlet. On the other hand, the relative concentration of colloids reaches zero at

approximately 15m from the fracture inlet since the curvature of the sinusoidal fracture increases the rate of diffusion of colloids into the rock matrix due to the high residence time available for the colloids in the fracture.
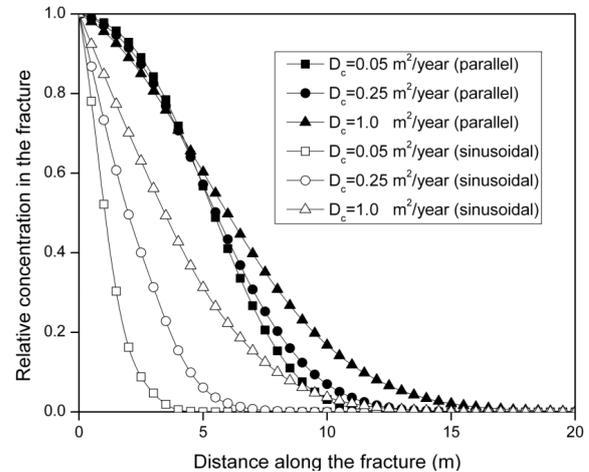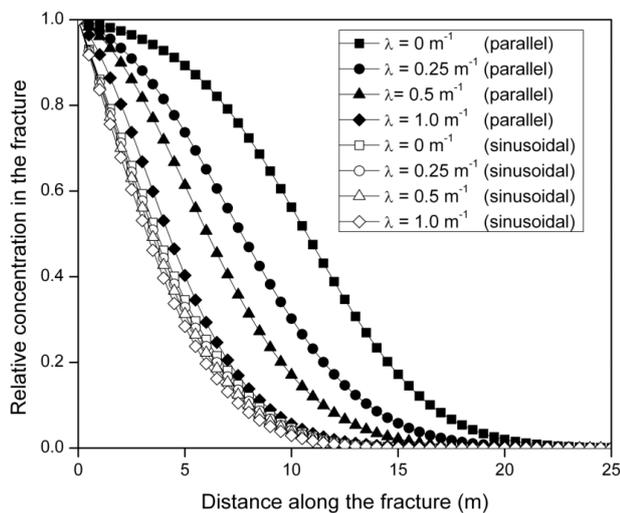

Figure 4. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models for various dispersion coefficients of colloids in the fracture. Refer Table 2 for base case parameters.

Figure 4 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal fracture model for various dispersion coefficients of colloids in the fracture. It is observed from Figure 4 that the concentration of colloids in the fracture increases with increase in the dispersion coefficient. The concentration profiles obtained from the parallel plate model for different dispersion coefficients merge with each other nearer to the fracture inlet due to the immediate diffusion of colloids into the rock matrix in all the cases and they deviate from each other far away from the fracture inlet. On the other hand, the concentration profiles obtained from the sinusoidal model for different dispersion coefficients are distinct from each other. This is because the fracture aperture in the sinusoidal fracture is varying spatially along the fracture as well as within the same cross section of the fracture. Thus, the behavior of the colloids movement within the fracture is distinct.

Figure 5. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models for various matrix porosities. Refer Table 2 for base case parameters.
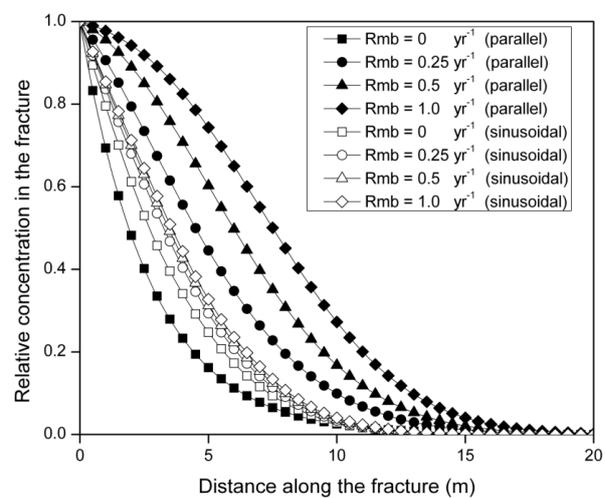
Figure 5 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal fracture model for various matrix porosities. It is observed from Figure 5 that both the colloids behave in the same manner for different matrix porosities in both the models. Due to the effect of the sinusoidal curvature of the fracture, the colloidal concentration in the sinusoidal fracture reaches zero at 15 from the fracture inlet while the concentration reaches zero at 20m from the fracture inlet in the parallel plate model.

Figure 6. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models for various filtration coefficients of colloids. Refer Table 2 for base case parameters.

Figure 6 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal
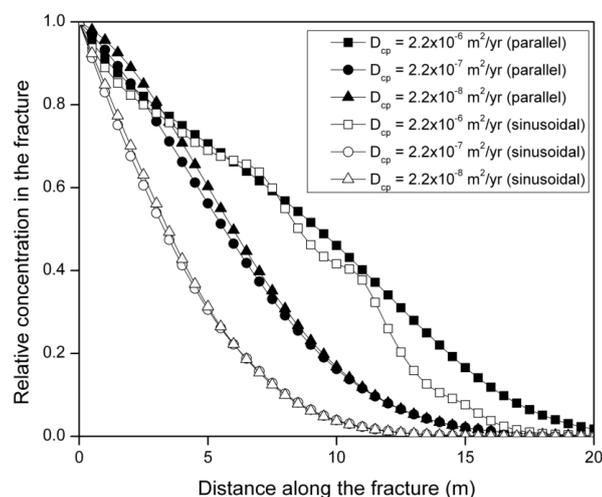
fracture model for various filtration coefficients of colloids. It is observed from Figure 6 that the concentration of colloids in the fracture reduces with increment in the filtration coefficient in the parallel plate model. This is because when the filtration coefficient is zero, i.e. $\lambda = 0$, none of the colloids are filtered from the aqueous phase and thus high concentration of colloids is observed in the fracture and on the other hand, when the filtration coefficient is very high all the colloids are filtered off from the aqueous phase resulting in very low concentration. In the sinusoidal fracture model, similar concentration profiles are observed for different filtration coefficients. This is because the zig zag nature of the fracture aperture hinders the filtration of colloids and thus increment in the filtration coefficient of colloids does not alter the concentration of colloids in the fracture.

Figure 7. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models for various remobilization coefficients of colloids. Refer Table 2 for base case parameters.

Figure 7 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal fracture model for various remobilization coefficients of colloids. It is observed from Figure 7 that the concentration of colloids in the fracture increases with increment in the remobilization coefficient in the parallel plate model. This is because when the remobilisation coefficient is zero, i.e. Rmb = 0, none of the colloids are remobilized back into the aqueous phase and thus very low concentration of colloids is observed in the fracture and on the other hand, when the remobilization coefficient is very high all the colloids are remobilized back to the aqueous phase resulting in high concentration. In the sinusoidal fracture model, similar concentration profiles are observed for different remobilization coefficients. The sinusoidal fracture does not enhance the remobilization of colloids into the aqueous phase which results in colloidal concentration reaching zero at the same distance from the fracture inlet for all the remobilization coefficients. In addition, it is assumed that 50% of the colloids are diffusing

into the rock matrix which also hinders the remobilization process.

Figure 8. Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models for various diffusion coefficients of colloids into the rock matrix. Refer Table 2 for base case parameters.

Figure 8 illustrates the comparison of concentration of colloids obtained from the parallel plate model and the sinusoidal fracture model for various diffusion coefficients of colloids into the rock matrix. In general, as the diffusion coefficient increases, the concentration of contaminants decreases in the fracture as more contaminants diffuse into the rock matrix. This phenomenon is observed nearer to the fracture inlet for very low diffusion coefficients for both the models and the profiles merge with each other father away from the fracture inlet. When the colloid diffusion coefficient is high, the colloidal concentration is significant in the fracture which is different from the usual behavior. In the parallel plate model, this phenomenon is observed because some of the colloids are filtered off from the aqueous phase which gets deposited on the fracture surface and only 50% of the colloids are assumed to enter the rock matrix. In the sinusoidal fracture model, the curvature of the fracture contributes to the non linear concentration profile of colloids and thus only a small fraction of the colloids are diffusing into the rock matrix.

V. CONCLUSION

Numerical simulation of colloidal transport in a sinusoidal fracture matrix coupled system has been attempted. The results suggest that the sinusoidal fracture model behaves differently from the parallel plate model. The concentration profiles obtained from the sinusoidal model for different dispersion coefficients are distinct from each other because the fracture aperture in the sinusoidal fracture is varying spatially along the fracture as well as within the same cross section of the fracture. Filtration and remobilization of colloids has negligible effect on the colloidal concentration in the sinusoidal fracture matrix system as the curvature of the

fracture aperture hinders the diffusion mechanism of the colloids. For high diffusion coefficients of the colloids, the concentration of colloids in the fracture is very significant which is different from the usual behavior resulting from the geometry of the fracture aperture and the proportion of colloids diffusing into the rock matrix.

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