Colloidal transport in a coupled fracture skin matrix system with sinusoidal fracture geometry

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Abstract— Colloidal transport in fractured media is a hot topic of research in nuclear engineering as colloids are carriers of radionuclides in the subsurface. A few studies have been conducted on colloidal transport in fractured matrix coupled system in the presence of fracture skin with parallel plate fracture model. An attempt has been made to simulate colloidal transport in sinusoidal fracture skin matrix coupled system numerically. Results suggest that the sinusoidal fracture model behaves differently from the parallel plate model as the fracture aperture is spatially varying. Filtration and remobilization of colloids has negligible effect on the colloidal concentration in the sinusoidal fracture matrix system in the presence of fracture skin.

Keywords— Colloidal transport, fracture skin, finite difference, remobilization, sinusoidal fracture

I. INTRODUCTION

Colloid transport in rock fractures is a very important phenomena as it enhances the contaminant transport in the subsurface media by acting as carriers for contaminants. 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; Kretschmar 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 exhaustive review on the occurrence of colloids, its

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properties and its transport in groundwater has been carried out by McCarthy and Zachara (1989).

Colloids are tiny particles in the size range of 1 nm to 1μm suspended in water, with high surface area and electrostatic charge (McCarthy et al. 1998a). 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 (McCarthy et al. 1998b). Colloids are present in the subsurface in the form of bacteria, viruses, metal oxides, clay minerals and humic macromolecules (Penrose et al. 1990; Short et al. 1998).

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.Significant research has been conducted on colloidal transport in fracture matrix coupled system while only a few of them address the transport of colloids in the fracture matrix system in the presence of fracture skin. Nair and Thampi (2010) developed a numerical model to describe the transport of colloids in a set of parallel fractures with fracture skin. Their model accounted transport of colloids along the fracture, irreversible deposition onto fracture surfaces, penetration into the rock formation, irreversible deposition onto the fracture skin surfaces and rock matrix surfaces. Natarajan and Suresh Kumar (2010a) developed a numerical model to describe the transport of colloid facilitated radionuclide transport in the fracture matrix system in the presence of fracture skin. They assumed that the radionuclides and the colloids are decay, sorb

onto the fracture surface, as well as diffuse into the fracture-skin and rock matrix. The sorption of the radionuclides onto the mobile and immobile colloids within the fracture is assumed to be linear. Nair and Thampi (2011) recently developed a   triple continuum one-dimensional transport model to analyse colloid facilitated contaminant transport in fractured geological formations. Their model accounts for contaminant transport in the fracture, reversible deposition onto fracture surfaces and onto the colloids, diffusion into the rock formation and irreversible deposition of colloids onto the fracture surfaces.

While most of these studies have been conducted on traditional parallel plate models, only a few studies have been conducted in irregular fractures with varying apertures. 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. 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 (2010b,c,d) have simulated solute transport, thermal transport and colloidal transport in a coupled sinusoidal fracture matrix system numerically. Natarajan and Suresh Kumar (2010e) have developed a numerical model for solute transport in a fracture matrix coupled system in the presence of fracture skin. None of the previous studies have attempted to analyse the transport of colloids in a coupled sinusoidal fracture matrix system in the presence of fracture skin. 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 in the presence of fracture skin. 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 fracture skin is considered to be one dimensional process.
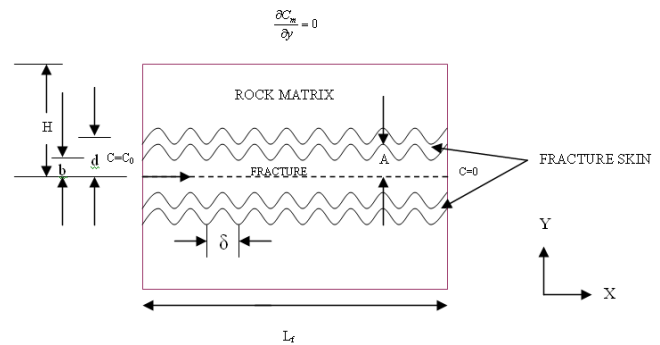

Fig. 1 Schematic diagram showing a coupled sinusoidal fracture-skin-matrix system

The assumptions regarding the geometry and hydrodynamic properties are as follows:
1. The fracture aperture 2b, is much smaller than the fracture length.
2. Advection is considered to be negligible in the fracture-skin and rock-matrix.
3. Transverse diffusion and dispersion within the fracture assures complete mixing across fracture widths at all times.
4. Permeability of the fracture-skin and rock-matrix is low, and molecular diffusion is assumed to be the main transport mechanism in them.
5. Transport along the fracture is much faster than transport in fracture-skin and rock-matrix.
6. Fracture, fracture-skin and rock-matrix are saturated.

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.

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

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

Q_C is the diffusion flux of the colloids from the fracture into the fracture skin and

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

ε is the percentage of matrix flux diffusion into the fracture skin 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 fracture skin and thus cannot diffuse into the fracture skin.

The governing equation for the colloid transport in the fracture skin is expressed as:

$$(1 + K_{d_{CP}})\frac{\partial C_P}{\partial t} - D_{CP}\frac{\partial^2 C_P}{\partial z^2} = 0 \tag{4}$$

$$x > 0, z \geq b, t \geq 0$$

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

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

$$(1 + K_{d_{CmatP}})\frac{\partial C_{mat}}{\partial t} - D_{Cmat}\frac{\partial^2 C_{mat}}{\partial z^2} = 0 \tag{5}$$

$$x > 0, z \geq b, t \geq 0$$

Where C_{mat} is the concentration of the colloids in the porous rock-matrix, D_{Cmat} is the dispersion coefficient of the colloids and $K_{d_{Cmat}}$ is the sorption partition coefficient for the colloids within the rock-matrix.

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

$C(x = 0, t) = C_0$ (6)

$C(x = L, t) = 0$ (7)

$C(x, t = 0) = C_P(x, z, t = 0) = C_{mat}(x, z, t = 0) = 0$ (8)

$C_P(x, z = b, t) = C(x, t)$ (9)

$C_p(x, z = d, t) = C_{mat}(x, z = d, t)$ (10)

$$\theta_P D_P \frac{\partial C_P(x, z = d, t)}{\partial x} = \theta_{mat} D_{mat}\frac{\partial C_{mat}(x, z = d, t)}{\partial x} \tag{11}$$

$$\frac{\partial C_{mat}(x, z = H, t)}{\partial z} = 0 \tag{12}$$

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 $5\times10^{-5}m^3$/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 in the presence of fracture skin. The numerical model using the conventional parallel plate fracture system without skin 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 is presented in Table 1. The results for the verification of the model have been shown in Figure 2.

Table I Parameters used for the validation of the numerical model for colloids

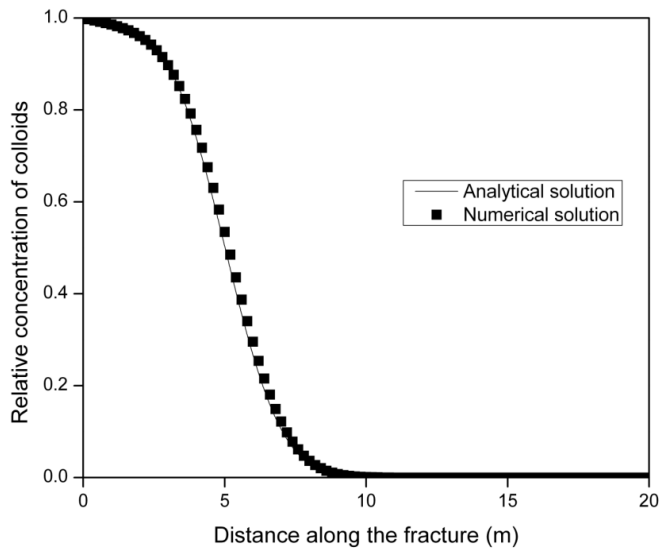| Parameter	Symbol	Value
Initial half-fracture aperture (m)	b	1.25e-04
Fluid velocity (m/year)	V	1
Hydrodynamic dispersion coefficient in the fracture (m^2/year)	D	0.25
Length of the fracture (m)	L_f	150
Total simulation time (day)	T	5
Colloid dispersion coefficient (m)	κ	1e-10
Concentration of colloids at the inlet of the fracture (kg/m^3)	C_o	1

Fig, 2 Validation of numerical results with analytical solution for colloid transport in a coupled fracture matrix system. 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. The parameters used for numerical simulation of colloid transport in the sinusoidal fracture skin matrix system are provided in Table 2.

Table II 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-matrix (m^2/year)	D_{CP}	2.2e-08
Distribution coefficient for colloids within the rock-matrix	$K_{d_{CP}}$	0.1
Distribution coefficient for colloids within the fracture skin	$K_{d_{Cmat}}$	0.1
Diffusion coefficient of colloids within rock matrix (m^2/year)	D_{Cmat}	4e-06
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
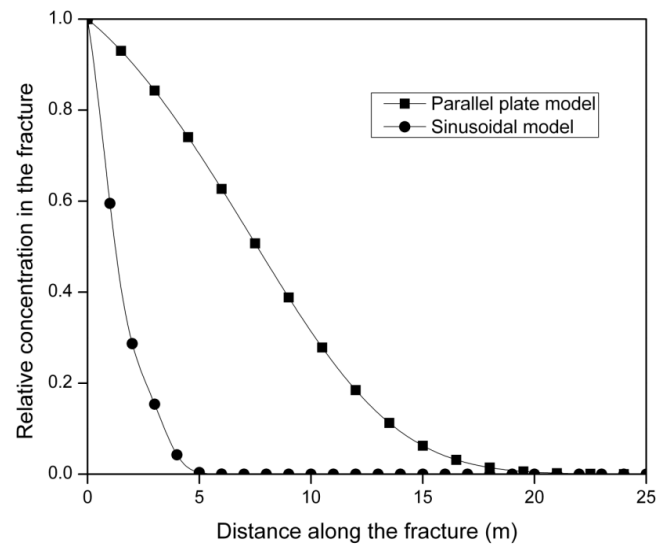
Fig. 3 Comparison of relative concentration of colloids obtained from parallel plate and sinusoidal fracture models. Refer Table 2 for base case parameters.

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 far away from the fracture inlet. On the other hand, the relative concentration of colloids reaches zero at approximately 5m from the fracture inlet in the sinusoidal fracture skin matrix system since the presence of skin in the sinusoidal fracture increases the rate of diffusion of colloids from the fracture to the rock matrix.
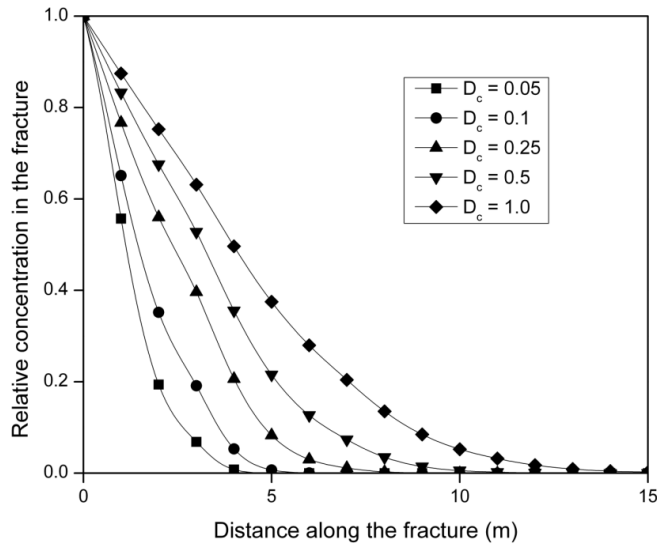

Fig. 4 Relative concentration of colloids obtained from sinusoidal fracture model for various dispersion coefficients of colloids in the fracture. Refer Table 2 for base case parameters.

Figure 4 illustrates the concentration of colloids obtained from 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 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. Due the varying cross section of the fracture aperture the dispersion of colloids increases with increase in dispersion coefficient.
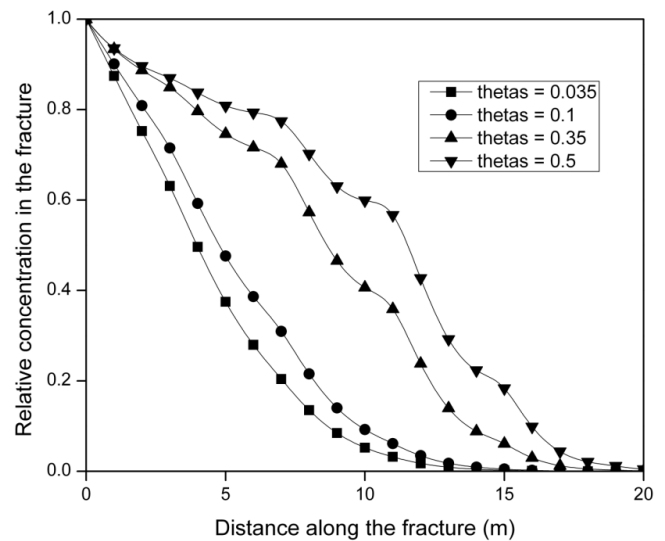

Fig. 5 Relative concentration of colloids obtained from sinusoidal fracture model for various fracture skin porosities. Refer Table 2 for base case parameters.

Figure 5 illustrates the concentration of colloids obtained from the sinusoidal fracture model for various fracture skin porosities. Generally, the concentration of colloids in the fracture decreases with increase in fracture skin porosities. It is observed in Figure 5 that the colloidal concentration increases with increment in fracture skin porosity. As skin porosity increases, more colloids are filtered off from the aqueous phase. This hinders further diffusion of colloids into the fracture skin. In addition, the remobilization of colloids and the varying fracture aperture also hinder the diffusion process.
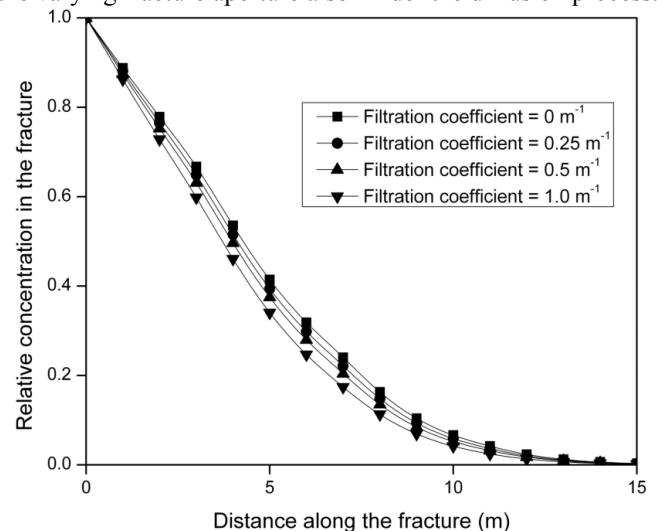

Fig. 6 Relative concentration of colloids obtained from sinusoidal fracture model for various filtration coefficients of colloids. Refer Table 2 for base case parameters.

Figure 6 illustrates the concentration of colloids obtained from 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. The colloidal concentration profiles are similar for all filtration coefficients.

This is because of the irregular nature of the fracture aperture which hinders the colloidal filtration and thus the variation of colloidal filtration coefficient has negligible effect on the concentration profile.
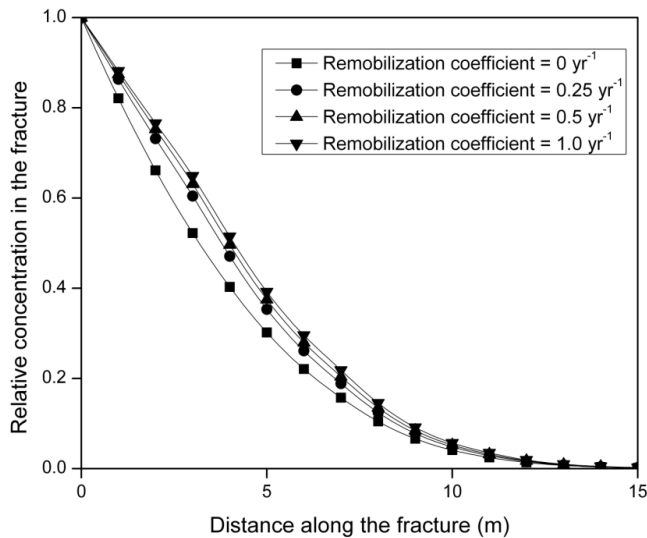

Fig. 7 Relative concentration of colloids obtained from sinusoidal fracture model for various remobilization coefficients of colloids. Refer Table 2 for base case parameters.

Figure 7 illustrates the concentration of colloids obtained from 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 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 except when the remobilization coefficient is one. The presence of fracture skin 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. The filtration colloids adsorbed on the sinusoidal fracture also interfere with the remobilization process.
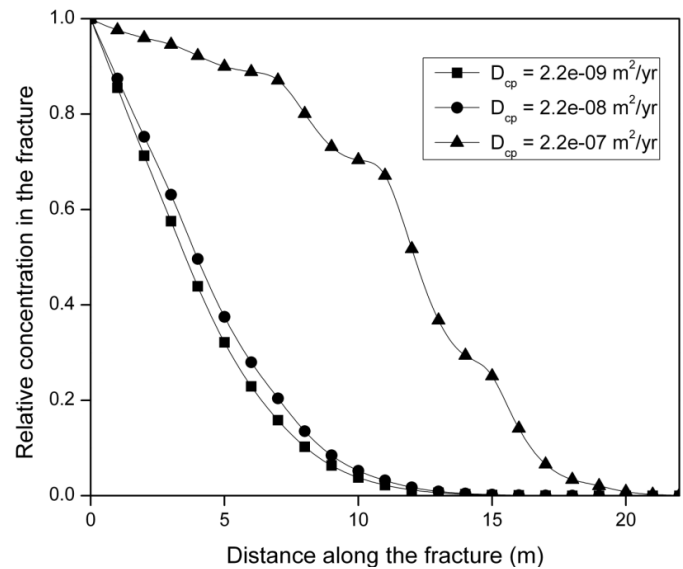

Fig. 8 Relative concentration of colloids obtained from sinusoidal fracture model for various diffusion coefficients of colloids into the fracture skin. Refer Table 2 for base case parameters.

Figure 8 illustrates concentration of colloids obtained from the sinusoidal fracture model for various diffusion coefficients of colloids into the fracture skin. In general, as the diffusion coefficient increases, the concentration of contaminants decreases in the fracture as more contaminants diffuse into the fracture skin. When the colloid diffusion coefficient is high, the colloidal concentration is significant in the fracture which is different from the usual behavior. The curvature of the fracture contributes retards the diffusion of colloids into the fracture skin.

V. CONCLUSION

Numerical simulation of colloidal transport in a sinusoidal fracture skin matrix coupled system has been attempted. 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 into the fracture skin. For high diffusion coefficients of the colloids, the concentration of colloids in the fracture is very significant which is different from the usual behavior due to combined effect of the fracture skin and the sinusoidal fracture aperture.

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