Modelling Equilibrium Colloid Deposition in Fractures with Fracture Skin

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Abstract — A fully implicit finite difference numerical model is developed for the transport of colloids in fractures with fracture skin. The conceptual model is developed based on the triple continuum approach. The model incorporates processes such as equilibrium colloid deposition onto the fracture surfaces, colloid penetration into the rock formation, sorption onto the fracture skin surfaces and sorption onto the rock matrix surfaces. Sensitivity analyses are performed to investigate the influence of various model parameters on the spatial evolution of colloid concentration in the fractured formation. It is demonstrated that the concentration of colloids along the fracture is influenced by the presence of fracture skin. It is also found that the colloid concentrations along the fracture increase with increase in size of colloids and increase in velocity.

Keywords — Colloid; Diffusion; Equilibrium Deposition; Fracture skin; Numerical model; Rock matrix; Sorption

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1 INTRODUCTION

Colloid transport in fractured formations has received considerable attention because of the potential role of colloids in facilitating the transport of pollutants, especially radionuclides, in the subsurface. Colloids are very fine particles that typically range in size between 1nm and 1μm [1]. Groundwater often contains significant populations of natural colloids which can interact with pollutants and influence their transport. Colloids may be introduced into or formed in subsurface water as a result of well drilling operations, through leachates from the vadose zone, and by dissolution of inorganic cementing agents that bind colloid-sized materials to the solid surfaces [2]. In fractured media, they are formed by the micro erosion of minerals present in the subsurface matrix as a result of formation crushing due to tectonic activity [3]. James and Chrysikopoulos [4] derived analytical solutions for monodisperse and polydisperse colloid transport in uniform fractures. Bradford and Torkzaban [5] reviewed pore-scale processes and models relevant for colloid transport and retention in unsaturated porous media. Several mathematical models have been developed to analyze the fate and transport of biocolloids and pathogens in subsurface environments [6], [7]. Analysis of colloid transport and colloid enhanced contaminant transport in subsurface formations are important as colloid particles serve as carriers of contaminants and significantly influence the net rate of contaminant migration.

Recently, it has been reported that the portions of the rock matrix adjacent to many open fractures are altered. These alterations are referred as fracture skins. Generally the transport properties of fracture skins are different from that of the undisturbed rock matrix and this, in turn, may influence contaminant transport through these formations [8]. Fracture skins are ubiquitous in nature and are especially noticeable in fractured formations where there is an interchange of fluids and solutes between the fractures and the matrix [8].

Zimmerman, Bennett and Sharp [9] examined the effect of sorption of organic solutes on altered fracture surfaces using an experimental fracture-flow apparatus. Garner and Sharp [10] investigated solute transport in granitic rocks with fracture skins at two climatically different field sites. Nair and Thampi [11] developed a numerical model for contaminant migration in fractures with fracture skin and analysed the influence of solute velocity on the transport of contaminant in fractured formations.

Most of the studies have employed dual continuum models, with the fracture and the rock matrix as two continums [12], [13] in the analysis of colloid transport in fractured formations. However, the presence of a fracture skin necessitates the application of a triple continuum approach in the analysis of transport of colloids in fractured formations. Till date, very few numerical models have been developed incorporating the fracture skin as a separate continuum for the analysis of colloid transport in fractures. In the present work, numerical models are developed based on the triple continuum concept to analyse the transport of colloids in fractured formations with fracture skin. The deposition of colloids onto the fracture surfaces is assumed to be governed by linear equilibrium isotherm assumption (LEA).

2 FORMULATION OF THE PROBLEM

A set of identical fractures (with fracture skin of constant thickness) whose axes are parallel and equally spaced is considered. The conceptualization of this fracture-skin- matrix system is shown in Fig. 1.

The following transport processes have been considered in this work: 1) advective transport along the fracture, 2) hydrodynamic dispersion within the fracture in the direction of the fracture axis, 3) diffusion-limited colloid transport at the fracture-skin interface, 4) adsorption onto the fracture wall, 5)

adsorption within the skin, 6) diffusion within the fracture skin, 7) adsorption within the matrix, and 8) diffusion within the matrix.
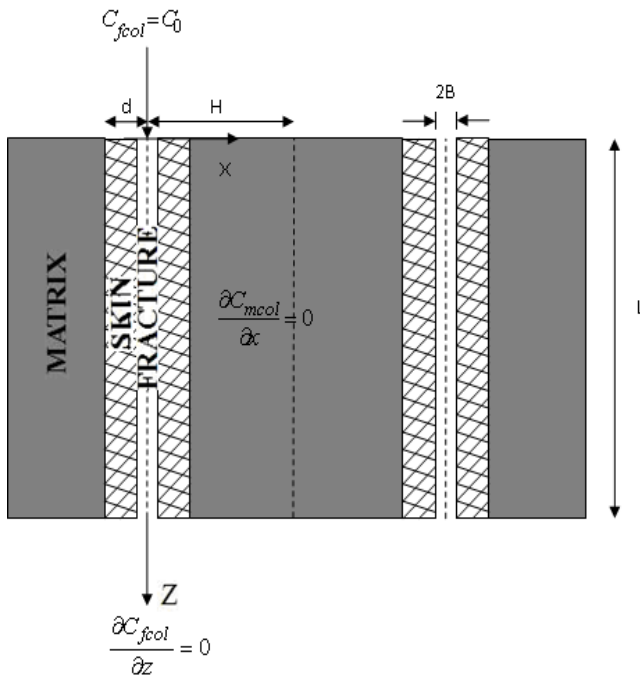

Fig. 1 Schematic representation of the fracture-skin-matrix system

Colloid transport processes in the fracture-skin-matrix system can be described by coupled one-dimensional equations for the fracture, the fracture skin and the matrix. The governing differential equation for transport of colloids in the fracture is based on the mass balance for an element in the fracture, assuming that colloids may deposit irreversibly onto the fracture surfaces and may penetrate the formation. This can be written as

$$\frac{\partial C_{fcol}}{\partial t} + \frac{1}{B}\frac{\partial C^*_{fcol}}{\partial t} = D\frac{\partial^2 C_{fcol}}{\partial z^2} - v\frac{\partial C_{fcol}}{\partial z} + \frac{\varphi_s}{B}D_{scol}\frac{\partial C_{scol}}{\partial x}\bigg|_{x=B} \quad (1)$$

where subscripts f, s and col denote the fracture, the skin and the colloids respectively, C_{col} is the aqueous concentration of the colloid (ML^{-3}), C^*_{fcol} is the concentration of colloids deposited onto fracture surfaces expressed as the mass of colloids per unit area of the fracture surface (ML^{-2}), v is the average linear groundwater velocity in the fracture (LT^{-1}), B is the half fracture aperture (L), D is the hydrodynamic dispersion coefficient (L^2T^{-1}), D_{scol} is the effective diffusion coefficient of the skin (L^2T^{-1}), and φ is the porosity. It may be noted that although the velocity distribution in the space between the two plates (idealization of the fracture aperture) is parabolic (Poiseuille flow) with zero magnitude at the fracture surfaces and a maximum magnitude of 1.5 times the average velocity midway between the two plates, in this work the velocity across the fracture width is assumed to be constant and equal to its vertically averaged magnitude.

The differential equation for transport of colloids in the fracture skin can be obtained in a similar manner, assuming that the interstitial liquid in the fracture skin is stationary and that colloids deposit irreversibly onto the fracture skin surfaces. The equation can be written as

$$\frac{\partial C_{mcol}}{\partial t} + \frac{\rho_m}{\varphi_m}\frac{\partial C^*_{mcol}}{\partial t} = D_{mcol}\frac{\partial^2 C_{mcol}}{\partial x^2} \quad (2)$$

Similarly, the governing differential equation for transport of colloids in the matrix is written as

$$\frac{\partial C_{mcol}}{\partial t} + \frac{\rho_m}{\varphi_m}\frac{\partial C^*_{mcol}}{\partial t} = D_{mcol}\frac{\partial^2 C_{mcol}}{\partial x^2} \quad (3)$$

The initial and boundary conditions to the problem can be stated as follows:

$$C_{fcol}(z,0) = C_{scol}(x,z,0) = C_{mcol}(x,z,0) = 0 \quad (4)$$

$$-D\frac{\partial C_{fcol}(0,t)}{\partial z} + vC_{fcol}(0,t) = vC_0 \quad (5a)$$

$$C_{fcol}(0,t) = C_0 \quad (5b)$$

$$\frac{\partial C_{fcol}(L,t)}{\partial z} = 0 \quad (6)$$

$$C_{fcol}(z,t) = C_{scol}(B,z,t) \quad (7)$$

$$\varphi_s D_{scol}\frac{\partial C_{scol}(d,z,t)}{\partial x} = \varphi_m D_{mcol}\frac{\partial C_{mcol}(d,z,t)}{\partial x} \quad (8)$$

$$C_{scol}(d,z,t) = C_{mcol}(d,z,t) \quad (9)$$

$$\frac{\partial C_{mcol}(H,z,t)}{\partial x} = 0 \quad (10)$$

3 NUMERICAL METHOD

The governing transport equations for the transport of colloids in a fracture-skin-matrix system are solved using a numerical model based on the finite difference method. A fully implicit numerical scheme is employed in formulating the numerical model. The advection part in (1) is discretised using an upwind implicit approach whereas the diffusion part is discretised using a fully implicit approach. The resulting set of simultaneous linear algebraic equations is solved using the Thomas algorithm. To ensure continuity of fluxes at the fracture – skin interface, the solution is iterated in each time step. A uniform grid size is selected along the fracture axis; finer grids are selected in the fracture skin whereas relatively larger grid sizes are adopted in the rock matrix. A relatively small

grid size at the fracture–skin interface helps to accurately compute the concentration flux into the fracture skin. Since analytical solutions are not available for transport of colloids in a fractured media with fracture skin, the performance of the numerical model is validated using the analytical solution for one dimensional colloid transport in fractured formations without fracture skin [12]. The computed results for this case are found to be in close agreement (Fig. 2) with the analytical solution of Abdel-Salam and Chrysikopoulos [12], indicating that the model developed is capable of analyzing the problem of colloid transport in a fractured media.
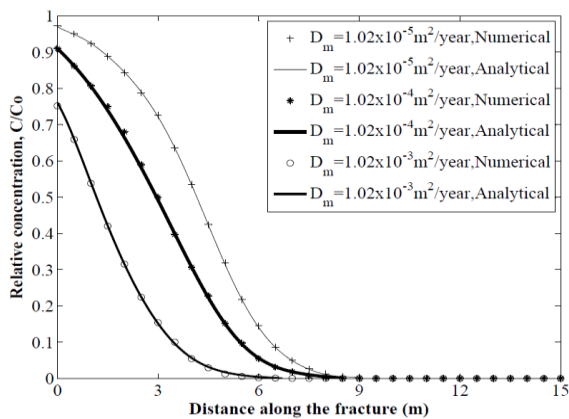

Fig. 2 Comparison of computed results with the analytical solution

Table 1 Input data for the base case

Parameters	Values
Average flow velocity in the fracture	1.0 (m/year)
Dispersion coefficient in the fracture	0.25 (m²/year)
Diffusion coefficient of skin	2.263×10^{-8} (m²/year)
Diffusion coefficient of matrix	1.504×10^{-9} (m²/year)
Porosity of skin	0.09
Porosity of matrix	0.024
Half fracture aperture	0.000565 m
Skin thickness	0.0207 m
Equilibrium distribution coefficient	3×10^{-7} m
Skin equilibrium distribution coefficient	0 (m³/ g)
Matrix equilibrium distribution coefficient	0 (m³/ g)
Fracture surface deposition coefficient	1×10^{-10} m
Fracture skin deposition coefficient	0 (year)⁻¹
Rock matrix deposition coefficient	0 (year)⁻¹
Fracture spacing	13.1 m
Density of colloidal particle	2×10^{6} (g/m³)

4 EQUILIBRIUM COLLOID DEPOSITION MODEL

The numerical model described in the previous section is used to simulate the transport of colloidal particles in a fractured formation. It is assumed that colloid deposition on the fracture surfaces is governed by the linear reversible equilibrium isotherm. The governing colloid transport equations in the fracture, the fracture skin and the rock matrix are represented by (1), (2) and (3) respectively. The mass flux of colloids deposited onto the fracture surfaces is represented by the second term on the left hand side of equation (1). Sorption of colloids onto the fracture surface is assumed to be governed by linear reversible isotherm and can be expressed as

$$C^{*}_{fcol} = K_{fcol} C_{fcol} \qquad (11)$$

where K_{fcol} represents the equilibrium distribution coefficient

Simulations are performed using the numerical model described above. The input data for the simulations are presented in Table 1. The concentration of colloids along the fracture, the fracture skin and the matrix are computed at the end of 5 years, assuming the length of the parallel fractures to be 300m. A detailed sensitivity analysis was performed to evaluate the influence of various colloid and fracture skin properties on colloid migration in a fractured media.

In order to illustrate the influence of fracture skin on colloid transport, concentration profiles along the fracture are computed for 'with skin' and 'no skin' conditions assuming the velocity of flow in the fracture as 1m/year. The results are presented in Fig. 3. It is evident from the results that the presence of fracture skin significantly influences the transport of colloid in fractured formations. The colloid concentration in the fracture is found to be lower in the presence of a fracture skin since larger amount of colloids is able to diffuse into it. Fig. 3 also demonstrates the influence of flow velocity on colloid transport in fractures. Simulations were performed at different flow velocities - 1m/year, 0.1m/year and 0.01m/year. The concentration profiles show that the increase in colloid penetration along the fracture is high at higher velocities. The results indicate that colloids penetrate a larger distance along the fracture at higher flow velocities. Also, the concentration profiles are similar for both boundary conditions except very close to the inlet boundary. The colloid concentration near the inlet boundary is steeply reduced at low flow velocities for a constant flux boundary condition. This can be attributed to the fact that a lower flow velocity results in smaller advective flux which in turn increases the diffusive flux of colloids in case of a constant flux inlet boundary case.

Fig. 4 demonstrates the influence of fracture skin porosity on colloid migration in fractures. ϕ is the relative porosity defined as the ratio of the fracture skin porosity to the rock matrix porosity. Computations were performed at three different relative porosity values- 0.375, 3.75 and 37.5. The plots

indicate that colloid concentrations along the fracture decreases as porosity of the fracture skin increases. This is because as the porosity of the skin increases, diffusion of colloids into the skin is enhanced.
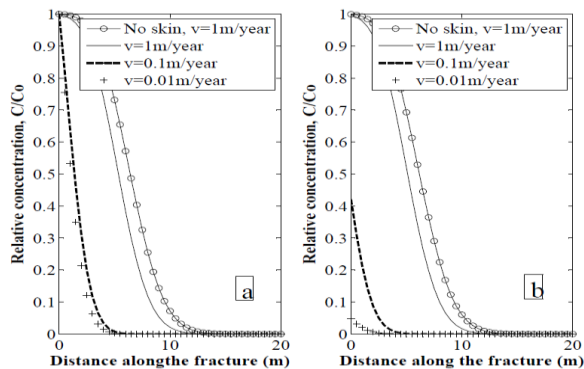

Fig. 3   Influence of flow velocity on colloid transport in a fracture (a) constant concentration at the inlet (b) constant flux at the inlet
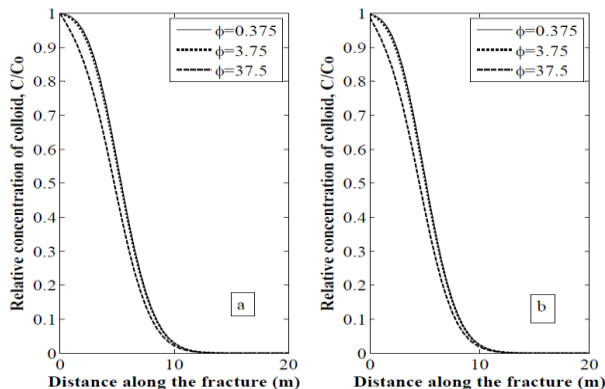

Fig. 4 Influence of skin porosity on colloid transport in a fracture a) constant concentration at the inlet b) constant flux at the inlet
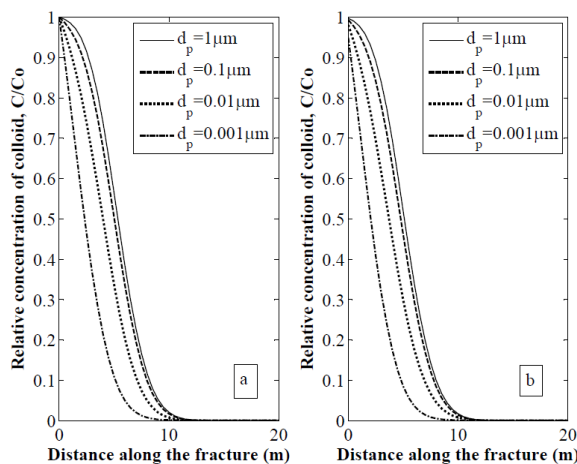

Fig. 5 Influence of size of colloids on colloid transport in fracture a) constant concentration at the inlet b) constant flux at the inlet

Fig. 5 demonstrates the influence of the size of colloids on colloid migration in a fracture for constant concentration and constant flux boundary conditions at the inlet. Simulations were carried out for different colloid sizes - 1μm, 0.1μm, 0.01μm and 0.001μm. Fig. 5 illustrates that a rapid increase in the concentration of colloids occurs between the 0.001μm and 0.1μm colloid sizes. As size of the colloidal particles increases, diffusion of colloids into the skin decreases, thereby increasing colloid concentrations along the fracture.

5   CONCLUSION

A numerical model is developed in a multiple continuum framework to analyze the problem of colloid transport in sets of parallel fractures with fracture skin. The model accounts for equilibrium colloid deposition onto the fracture surfaces, penetration into the fracture skin and the rock matrix, and deposition onto the fracture skin and the rock matrix surfaces. Colloid transport processes in the fractured formation are described by coupled one-dimensional equations for the fracture, the fracture skin and the matrix. The set of coupled partial differential equations are discretised using a fully implicit numerical formulation. Sensitivity analyses are performed to investigate the influence of colloid velocity, fracture skin porosity and colloid size on the spatial evolution of colloid concentration in the fractured formation.

It can be concluded that the presence of fracture skin influences the transport of colloids in the fracture. It is also found that the colloid concentrations along the fracture increases with increase in size of colloids and increase in colloid velocity.

The study underlines the importance of the triple continuum approach for modelling colloid transport in a saturated, fracture-skin-matrix coupled system. The model results are useful in characterization studies of colloid transport in fractured formations with fracture skin and have implications on efforts for better remediation of groundwater quality.

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