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Numerical modelling of colloidal transport in fractured porous media with double layered fracture-skin

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Abstract. A numerical model is developed for studying the transport of colloids in a coupled fracture-matrix system with double layer fracture-skin. The governing equations describing colloid transport along the fracture and diffusion into fracture-skin layers as well as rock-matrix, normal to the fracture axis are coupled with each other. The coupled non linear equations are solved numerically with fully implicit finite difference method. Sensitivity analysis is performed to investigate the effect of various colloid properties on the colloid concentration in the multiple porosity fractured system. Colloid remobilisation and filtration has been accounted in the model. Results suggest that the inclusion of a second fracture-skin layer has a marginal effect on the transport mechanism of colloids. As colloid velocity increases, the diffusion of colloids into the fracture-skin decreases due to the low residence time available for the colloids. High first layer fracture-skin thickness and porosity enhances the diffusion of colloids from the aqueous phase of the fracture into the skin considerably resulting in low colloidal concentration within the fracture. Variation in the fracture. The colloid transport mechanism in fractured porous media is marginally affected by the multiple porosity system, or in other words additional layers of fracture skin. High filtration coefficient and low remobilisation coefficient result in low colloidal concentration within the fracture.

Keywords: Fracture, double layered skin, colloid, remobilisation, filtration

1.. Introduction

Colloidal transport in fractured porous media is an important area of research because of the ability of colloids in facilitating the transport of contaminants in the subsurface. Earlier studies have reported the adsorption of contaminants on colloids and thus enhancing the mobility of contaminants in fractures [4–6, 8, 13, 15, 16, 26, 27, 29, 30]. Colloids are tiny particles in the size of 1 nm to 1 μ m suspended in water, with high surface area and electrostatic charge [9]. Colloids are present in the subsurface in the form of bacteria, viruses, metal oxides, clay minerals and humic macromolecules [Mills et al., 1991; 17].

Significant research has been carried out on the transport of colloids in fractured porous media. Hwang et al. [10] presented a model for colloid migration in a single planar fracture with the assumption that the colloids are not depositing on the fracture surfaces. Abdel-Salam and Chrysikopoulos [3] presented an analytical solution for transport of colloids in a single fracture for constant concentration as well as constant flux boundary conditions.

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It should be noted however that Abdel-Salam and Chrysikopoulos [1, 2] have shown that depending on the nature of the colloids and the physical conditions of the fractured system, colloids can enhance or hinder the mobility of contaminants. Chrysikopoulos and Abdel-Salam [7] developed a numerical model to describe colloidal transport in a saturated fracture with spatially variable aperture under various physicochemical conditions, accounting for the deposition of colloids on fracture surfaces. James and Chrysikopoulos [11] derived analytical solution for transport of monodisperse and polydisperse colloids in a uniform fracture. James and Chrysikopoulos [12] developed a particle tracking numerical model to examine the effect of gravity on monodisperse and polydisperse colloids transport in fractures, and concluded that larger dense colloid particles spread over wider sections of the fracture along the flow direction, but smaller particles travel slower or faster than the larger particles depending on the fracture orientation angle. Recent investigations have strongly suggested the role of fracture-skin at fracture-matrix interface, whose rock properties are generally found to be significantly different from that of its associated rock-matrix [25].

Therefore, the nature of diffusive mechanisms is different at the fracture-skin interface as well as at the skinmatrix interface. Diffusive transport at the fracture-skin interface results from transfer of solutes from mobile fluid in the fracture to immobile fluid within the fracture-skin, while the diffusive transport at the skin-matrix interface results from transfer of solutes within immobile fluids, and leads to differing diffusion rates [24]. As a consequence, the mechanism of colloid transport across the fracture-skin interface would be quite different from that of the conventional fracture-matrix interface. Nair and Thampi [20] have developed a numerical model to describe the transport of colloids in sets of parallel fractures with fracture-skin. They performed sensitivity analysis to investigate the effect of various colloid properties on the evolution of colloid of colloid concentration in the fractured formation with fracture-skin. Natarajan and Suresh Kumar [21] developed a numerical model for studying the transport of colloids accompanied by radionuclides in a coupled fracture-skin-matrix system. Nair and Thampi [20] developed a numerical model to analyse colloid facilitated contaminant transport in the fractured porous media with fracture-skin. Natarajan and Suresh Kumar [22] developed a numerical model for describing the transport of virus in a fracturematrix system in the presence of fracture-skin. Natarajan and Suresh Kumar [23] also investigated the evolution of fracture permeability in a coupled fracture matrix system in the presence of fracture-skin with simultaneous colloidal and bacterial transport, by taking into account the effects of thermal stress and silica precipitation/dissolution. From literature, it is evident that modelling studies on the colloidal transport in fractured media with fracture-skin is limited.

As mentioned earlier the formation of fracture skin can significantly influence the colloid transport mechanism in fractured porous media due to its distinctive properties compared to that of the rock matrix. Literature shows that the earlier studies conducted on colloid transport in fractured porous media pertain only to single layer of fracture skin. The formation of multiple layers of fracture skin in fractured porous media is also feasible phenomena as formation of fracture skin is expressed by Robinson et al. [25] as a process of exchange of solutes and minerals between the fracture and the rock matrix. Therefore, this study plays a major role in understanding the impact of additional layers of fracture skin on the colloidal transport mechanism in fractured porous media. In this study, an attempt has been made to analyse the transport of colloids in fractures with double layer fracture-skin or in other words a multiple porosity system.

2. Physical system and governing equations

The conceptual model corresponding to a coupled fracture-skin-matrix system is illustrated in Fig. 1. In Fig. 1, b represents the half fracture aperture, d_1 -b represents the thickness of the first layer of fracture-skin, d_2 -b represents the thickness of the second layer of fracture-skin H represents the thickness of the half fracture spacing.

The assumptions regarding the geometry and hydrodynamic properties are as follows:

- 1. The fracture aperture 2b, is much smaller than the fracture length.
- 2. Fracture walls are smooth and parallel plate assumption is considered for modelling transport in the fracture.
- 3. Advection is considered to be negligible in the fracture-skin and rock-matrix.
- 4. Transverse diffusion and dispersion within the fracture assures complete mixing across fracture widths at all times.



Fig. 1. Schematic representation of a fracture-matrix coupled system with double layer of fracture-skin.

- 5. Permeability of the fracture-skin and rock-matrix is low, and molecular diffusion is assumed to be the main transport mechanism in them.
- 6. Transport along the fracture is much faster than transport in fracture-skin and rock-matrix.
- 7. Fracture, fracture-skin and rock-matrix are saturated.
- 8. Width of fracture is assumed to be much smaller than the length of the fracture.
- 9. Porosity in the fracture is 100 percent.
- 10. Only the averaged fluid velocity along the longitudinal direction of the fracture has been considered in this study as the fracture aperture is very small compared to the length of the fracture.

The governing equation for the colloid transport in the fractured porous media has been adopted from Li et al. [14]. The equations and boundary conditions have been modified to take into account of the second fracture-skin layer. The governing equation for colloidal transport in the fracture is given by:

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

where C is the colloidal concentration in the fracture, σ_c is the concentration of colloids attached to the fracture wall surface (immobile colloids), V_c is the velocity of the colloids, D_c is the dispersion coefficient of colloids, b is the half fracture aperture. The governing equation for immobile colloids is given as:

$$\frac{\partial \sigma_C}{\partial t} = \lambda_f V_C C b - R m b \sigma_c \tag{2}$$

where λ_f is the colloid filtration coefficient, *Rmb* is the colloid remobilisation coefficient., *b* is the half fracture aperture.

In Equation 1, Q_C is the diffusion flux of the colloids from the fracture into the fracture-skin

$$Q_C = -\varepsilon \theta_{P1} D_{CP1} \frac{\partial C_{P1}}{\partial z} \bigg|_{z = b}$$
(3)

 ε is the percentage of 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 cannot diffuse into the fracture-skin, θ_{CP1} is the porosity of the first porous fracture skin layer, D_{CP1} is the diffusion coefficient of colloids into the first porous fracture skin layer, C_{P1} is the concentration of colloids in the first porous fracture skin layer.

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

$$(1+K_{dCP1})\frac{\partial C_{P1}}{\partial t} - D_{CP1}\frac{\partial^2 C_{P1}}{\partial z^2} = 0$$

$$\tag{4}$$

where C_{P1} is the concentration of the colloids in the first porous fracture-skin layer, D_{CP1} is the diffusion coefficient of the colloids into the first skin layer and $K_{d_{CP1}}$ is the sorption partition coefficient for the colloids within the first fracture-skin layer.

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

$$(1 + K_{d_{CP2}})\frac{\partial C_{P2}}{\partial t} - D_{CP2}\frac{\partial^2 C_{P2}}{\partial z^2} = 0$$
(5)

where C_{P2} is the concentration of the colloids in the second porous fracture-skin layer, D_{CP2} is the diffusion coefficient of the colloids into the second skin layer and $K_{d_{CP2}}$ is the sorption partition coefficient for the colloids within the second fracture-skin layer.

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

$$(1 + K_{d_{Cmat}})\frac{\partial C_{mat}}{\partial t} - D_{Cmat}\frac{\partial^2 C_{mat}}{\partial z^2} = 0$$
(6)

where C_{mat} is the concentration of the colloids in the porous rock-matrix, D_{Cmat} is the diffusion 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:

$$C(x = 0, t) = C_0 \tag{7}$$

$$C(x = L, t) = 0 \tag{8}$$

$$C(x, t = 0) = C_{P1}(x, z, t = 0) = C_{mat}(x, z, t = 0) = C_{P2}(x, z, t = 0) = 0$$
(9)

$$C_{P1}(x, z = b, t) = C(x, t)$$
 (10)

$$C_{p1}(x, z = d_1, t) = C_{P2}(x, z = d_1, t)$$
 (11)

$$C_{p2}(x, z = d_2, t) = C_{mat}(x, z = d_2, t)$$
 (12)

$$\theta_{P2}D_{P2}\frac{\partial C_{P2}(x,z=d_2,t)}{\partial z} = \theta_{mat}D_{mat}\frac{\partial C_{mat}(x,z=d_2,t)}{\partial z}$$
(13)

$$\theta_{P2}D_{P2}\frac{\partial C_{P2}(x,z=d_1,t)}{\partial z} = \theta_{P1}D_{P1}\frac{\partial C_{P1}(x,z=d_1,t)}{\partial z}$$
(14)

$$\frac{\partial C_{mat}(x, z = H, t)}{\partial z} = 0 \tag{15}$$

where Co is the concentration of the colloids at fracture inlet.

3. Numerical model

In this study, the system is described by a set of four partial differential equations for colloids; one for the fracture, another for first fracture-skin layer, another for second fracture-skin layer and another for the rock-matrix formulated for a one-dimensional framework. The continuity at the fracture and fracture-skin interface is attained by iterating the solution at each time step. The coupled system is solved numerically using implicit finite difference scheme. The advection part is discretised using Upwind scheme and the diffusion part using second order central difference scheme. A varying cell width is adopted in the first fracture-skin layer. A smaller grid size is adopted in the fracture and fracture-skin interface to accurately capture the flux transfer.

The last term on the left hand side of Equation (1) which accounts for the flux diffusion from the fracture into the first layer of the fracture skin is discretised as

$$\frac{\partial C_{P1}}{\partial z} = \frac{C_{P1}^{n+1} - C_{P1}^{n+1}}{\Delta z(1)}$$
(16)

where $\Delta z(1)$ represents the cell width across the fracture-skin interface. Here the concentration in the first node in the fracture skin, i.e., C_{P1}^{n+1} will be equal to the corresponding fracture concentration $C^{n+1}_{1}\Big|_{i=1}^{n}$ thereby

satisfying the boundary condition provided in Equation (10).

The concentration at the second node of the first layer of the fracture skin C_{p1}^{n+1} is the fourth unknown in in Equation (1). The value of this unknown is assumed and Equation (1) is solved to obtain the fracture concentration. This fracture concentration is used as the boundary condition for the first layer of the fracture skin as indicated in Equation (11). The colloidal concentration for the first layer of the fracture skin is calculated using Equation (4). This new first layer fracture skin concentration is now compared with the initially assumed fracture skin concentration. If the difference between both the concentrations exceeds the assumed tolerance limit, the new fracture skin concentration is used for solving Equation 1 again, to obtain the fracture concentration. The above process is repeated until the convergence of the first layer of the fracture skin and the rock matrix are obtained using Equations (5) and (6) taking into account of the boundary conditions provided in Equations (11) and (12). The fracture skin and rock matrix concentrations obtained within a time step is used for the next time step. Thus, using tridiagonal matrix algorithm (TDMA), the three unknowns are solved for the fracture at ith node, (i + 1)th node at (n + 1)th time level.

4. Results and discussion

The influence of double layered fracture-skin on the transport of colloids in a fractured matrix coupled system is analyzed. For the purpose of verification of the numerical model, the concentration profiles of the colloids have been computed using a Direchlet type boundary condition at the inlet as well as the outlet of the fracture. The result of the numerical model for colloids in a single fracture is compared with the analytical solution of Van Genuchten [28]. The parameters used for validation of the numerical results with the analytical solution for radionuclides and colloids are presented in Table 1.

The result for the verification of the model has been shown in Fig. 2. The analytical solution is represented by solid lines while the numerical solution is represented by data points.

It is observed from Fig. 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 colloidal transport in fracture matrix coupled system with double layered fracture-skin are presented in Table 2 below.

Figure 3 represents the spatial distribution of relative concentration of colloids for different colloid velocities. It is observed from the figure that when the colloidal velocity is low, the colloidal concentration in the fracture becomes zero close to the fracture inlet. This is because the residence time available for the colloids in the fracture

Farameters used for the varidation of the numerical model for conolds			
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)	Т	5	
Colloid dispersion coefficient (m)	κ	1e-10	
Concentration of colloids at the inlet of the fracture (kg/m^3)	Co	1	

Table 1 Parameters used for the validation of the numerical model for colloids



Fig. 2. Validation of numerical results with analytical solution for colloid transport in a single rock fracture (Refer to Table 1 for data).

 Table 2

 Parameters for colloidal transport in fractured porous media with double layered fracture-skin

Parameter	Symbol	Value
Initial half-fracture aperture (m)	b	200e-06
First fracture-skin thickness (m)	d ₁ -b	0.002
Second fracture-skin thickness (m)	d2-d1	0.001
Average fluid velocity (m/d)	V _C	1
Porosity of the first fracture-skin layer	$\theta_{\rm P1}$	0.035
Porosity of the second fracture-skin layer	θ_{P2}	0.235
Porosity of the rock matrix	$ heta_{ m m}$	0.645
Total simulation time (day)	Т	10
Length of the fracture (m)	L_{f}	50
Remobilisation coefficient for colloids (yr^{-1})	Rmb	0.5
Filtration coefficient for colloids (m^{-1})	λ_{f}	0.5
Percentage of diffusion for colloids	ε	0.5
Diffusion coefficient of colloids within the first fracture-skin layer (m ² /d)	D _{CP1}	2.2e-08
Diffusion coefficient of colloids within the second fracture-skin layer (m ² /d)	D _{CP2}	2.2e-05
Diffusion coefficient of colloids within the rock-matrix (m^2/d)	D _{Cmat}	4e-06
Diffusion coefficient for colloids within the first fracture-skin layer (m ² /d)	$K_{d_{CP1}}$	0.5
Diffusion coefficient for colloids within the second fracture-skin layer (m ² /d)	K _{dCP2}	0.5
Diffusion coefficient for colloids within the rock-matrix (m ² /d)	K _{dCmat}	0.1
Remobilisation coefficient for colloids in the fracture (d^{-1})	Rmb	0.5
Dispersion coefficient of colloids within the fracture (m ² /d)	D	1e-06



Fig. 3. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different colloid velocities. Refer to Table 2 for other data.



Fig. 4. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different first layer fracture-skin porosities. Refer to Table 2 for other data.

is high which allows considerable time for them to diffuse into the adjacent fracture-skin layer. As the velocity of colloids is increased, the colloidal concentration in the fracture increases.

Figure 4 represents the spatial distribution of relative concentration of colloids for different first layer fractureskin porosities. It is observed from Fig. 4 that the concentration profiles is the same for all the cases at the inlet of the fracture but as the colloids are transported along the fracture, the profiles vary for different fracture-skin porosities. The colloidal concentration along the fracture is low for high fracture-skin porosity. As the first layer skin porosity is reduced, the concentration of the colloids along the fracture increases. Thus, high skin porosity enables considerable diffusion of colloids into the fracture skin and thereby reduces the concentration along the fracture. The presence of fracture-skin consequently aids in the reduction of colloid facilitated contaminants within the fractured porous media as reported by Natarajan and Suresh Kumar [21].

Figure 5 represents the spatial distribution of relative concentration of colloids for different second layer fractureskin porosities. It is observed from Fig. 5 that there is no variation in the colloid concentration profiles for different second layer fracture-skin porosities. This shows that in a multiple porous fractured system, the porosity of the skin layer adjacent to the fracture plays a major role compared to one located below the first layer.

Figure 6 represents the spatial distribution of relative concentration of colloids for different rock-matrix porosities. It is observed from Fig. 6 that there is no variation in the colloid concentration profiles for different rock-matrix porosities when there are double fracture-skin layers. The fracture-skin layers impede the diffusion of colloids



Fig. 5. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different second layer fracture-skin porosities. Refer to Table 2 for other data.



Fig. 6. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for rock-matrix porosities. Refer to Table 2 for other data.

into the rock-matrix and therefore varying the rock-matrix porosity does not have any influence on the colloidal concentration within the fracture.

Figure 7 represents the spatial distribution of relative concentration of colloids for various first layer fracture-skin thicknesses. It is observed from Fig. 7 that when the fracture-skin thickness is high; the colloidal concentration along the fracture reduces considerably as the high skin thickness enhances the diffusion of colloids from the fracture. On the other hand, when the fracture-skin thickness is low, the colloidal concentration reaches zero at the farther end of the fracture. When the fracture-skin thickness is low, the effect of filtration as well as remobilisation is enhanced. The filtered colloids are remobilised into the aqueous phase easily resulting in high colloidal concentration along the fracture. Moreover, as observed in Fig. 5 the influence of second layer fracture-skin thickness is low, which causes the concentration to be high for major portion of the domain before the concentration reduces to zero.

Figure 8 represents the spatial distribution of relative concentration of colloids for various second layer fractureskin thicknesses. It is observed from Fig. 8 that the colloidal concentration profile remains the same for different second layer fracture-skin thicknesses.

Figure 9 represents the spatial distribution of relative concentration of colloids for various colloid filtration coefficients. It is observed from Fig. 9 that when the filtration coefficient is high, the colloidal concentration along the fracture is low. This is because large quantum of colloids is filtered off from the aqueous phase into the fracture-skin. As the filtration coefficient is reduced, the concentration of colloids within the fracture increases. It is well



Fig. 7. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different first layer fracture-skin thicknesses. Refer to Table 2 for other data.



Fig. 8. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different second layer fracture-skin thicknesses. Refer to Table 2 for other data.

known that the colloidal transport mechanism is quite different from the solute transport mechanism. Even though the porosity of the first fracture skin layer is low compared to the second layer and the rock matrix, the filtration coefficient plays an important role in the removal of colloids from the aqueous phase and thus influences the colloid concentration within the fracture.

Figure 10 represents the spatial distribution of relative concentration of colloids for various colloid remobilisation coefficients. It is observed from Fig. 10 that when the remobilisation coefficient is high, the colloidal concentration along the fracture is high. This is because large quantum of colloids is remobilised back into the aqueous phase from the fracture-skin. As the remobilisation coefficient is reduced, the concentration of colloids within the fracture decreases. Remobilisation of colloids into the aqueous phase of the fracture is an important feature of the colloid transport mechanism as the filtered colloids return back to the system depending on the physical and chemical conditions. This can also enhance the mobility of contaminants in fractured porous media as they aid the mobility of contaminants through sorption [19, 21].

Figure 11 represents the spatial distribution of relative concentration of colloids for various colloid diffusion coefficients into the fracture-skin. It is observed from Fig. 11 that for low diffusion coefficients, the colloidal concentration along the fracture remains high for major portion of the domain before it becomes zero at the farther end of the fracture. On the other hand, high diffusion coefficients lead to considerable diffusion of colloids into the fracture-skin, resulting in low concentration within the fracture.



Fig. 9. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different colloid filtration coefficients. Refer to Table 2 for other data.



Fig. 10. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different colloid remobilisation coefficients. Refer to Table 2 for other data.



Fig. 11. Spatial distribution of relative concentration of colloids in a multiple porous fractured system for different colloid diffusion coefficients into the fracture-skin. Refer to Table 2 for other data.

5. Conclusions

A numerical model is developed to analyse the transport of colloids in a coupled fracture-matrix system with double fracture-skin layer, i.e., multiple porous fractured system. The set of coupled equations for colloidal transport in fracture-skin-matrix system is solved using implicit finite difference method. Constant continuous source of colloids is assumed at the inlet of the fracture. A sensitivity analysis is performed to investigate the effect of various colloid transport parameters on the colloidal concentration in the multiple porous fractured system.

The presence of second layer of fracture-skin has a marginal effect on the colloidal transport mechanism. As the colloid velocity increases, the diffusion of colloids into the fracture-skin decreases as the residence time available for the colloids is decreased. High fracture-skin porosity enables high diffusion of colloids from the fracture into the fracture-skin resulting in low colloidal concentration within the fracture. The colloidal concentration remains unaffected for different rock-matrix porosities and second layer fracture-skin porosities. Thus, in a multiple porous fractured system, the fracture-skin adjacent to the fracture has major influence on the colloidal transport mechanism.

Further, increment in the fracture-skin thickness (first layer) enhances the diffusion of colloids from the fracture resulting in low colloidal concentration within the fracture. The colloidal concentration remains unaffected for variations in the thickness of the second layer of fracture-skin thickness. As the filtration coefficient is increased the colloidal concentration in the fracture is decreased as more colloids are filtered from the aqueous phase. The reverse mechanism occurs in the case of remobilization coefficient. The effect of colloidal diffusion coefficient into the fracture-skin on colloid migration was analyzed. It is observed that as the diffusion coefficient is increased the colloidal concentration in the fracture decreases.

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