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Original Article

Effect of time varying fracture skin porosity on the contaminant transport mechanism in fractured porous media

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Abstract

In this paper, the effect of time varying fracture skin porosity on the contaminant transport mechanism in the fractured porous media is analyzed using numerical modeling. An implicit finite difference numerical technique has been used to solve the coupled non-linear governing equations. The effect of increasing porosity with time on the contaminant transport mechanism has been analyzed for various initial fracture skin porosities. Results suggest that time varying fracture skin porosity can affect the contaminant transport mechanism in a fracture matrix coupled system The concentration rapidly reduces within the fracture for various half fracture apertures and fracture-skin diffusion coefficients due to the effect of time varying fracture-skin porosity.

Keywords: fracture, fracture-skin, time varying skin porosity, contaminant transport, rock matrix

1. Introduction

Study on fluid flow and contaminant transport through fractured porous media has gained considerable interest in the recent decades as fractures form a source of preferential pathways in the subsurface media. Fractures play a major role in different systems like geothermal, petroleum, oil and gas, radioactive repositories and so on. Consequently, understanding the mechanism of transport in fractures plays a crucial role for the hydrogeologists. The most important aspect of transport of contaminants in fractured media is how the exchange of solutes and fluids takes place between the fracture and the surrounding rock matrix.

Extensive research has been conducted on transport of contaminants in fractured media considering the same to be a dual porosity system (Bear *et al*., 1993; Evans & Nicholson, 1987; Grisak & Pickens, 1980; Haggerty *et al*., 2000; Maloszewski & Zuber, 1985, 1990; Natarajan & Suresh Kumar, 2011a, 2011b, 2011c, 2012a, 2015, 2016a; Ota *et al*., 2003; Polak *et al*., 2003; Rasmuson, 1984; Raven *et al*., 1988; Sudicky & Frind, 1982; Suresh Kumar, 2008, 2009; Suresh Kumar & Sekhar, 2005; Suresh Kumar *et al*., 2011; Sekhar *et al*., 2006; Tang *et al*., 1981; Wallach & Parlange, 1998).

Recent investigations have revealed the formation of an additional low permeability layer known as the fracture skin in many hydraulically active near surface fractures (Kreisel & Sharp, 1996; Robinson *et al*., 1998; Sharp, 1993). The presence of fracture skin results in a triple continuum system, i.e., fracture, fracture skin and rock matrix. Fracture skins are defined as low permeability material, deposited along the fracture walls, and subsequently mitigates the diffusive mass transfer between the high as well as low permeability materials (Moench, 1984, 1995). The skin consists of clay minerals, organic matter, as well asiron and manganese oxides (Fu *et al*., 1994), which are considered to be potential absorbers. While a few studies have reported a reduction in the permeability of the fracture skin (Deiese *et al*., 2001; Fu *et al*., 1994; Robinson & Sharp, 1997) some others have reported an increment in the permeability of the fracture skin (Polak *et al*., 2003). This basically depends on the material that is being deposited on the fracture walls which forms the fracture skin. Fu *et al*. (1994) have demonstrated that the weathering rinds have provided a significant increase in porosity of the fracture skin with that of the

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associated rock matrix porosity. As the properties of the fracture skin are completely different from that of the rock matrix, the fracture skin can significantly affect the diffusive mechanisms at the fracture-skin interface as well as the skin-matrix interface. Thus, formation of fracture skin can either enhance or mitigate the mass transfer at the interface of the fracture and the rock matrix (Robinson *et al*., 1998).Studies have been conducted on transport of contaminants through fractured porous media with skin formation (Nair & Thampi 2010; 2011; Natarajan, 2014; Natarajan & Suresh Kumar, 2010, 2012b, 2012c, 2012d, 2012e, 2014a; 2014b, 2016b; Renu & Suresh Kumar, 2012, 2014;).

In all the above studies, the authors have considered the fracture-skin porosity to be constant during the simulation period. There is evidence of variation of porosity of the porous media due to bioclogging from literature (Brovelli *et al*., 2009; Ham *et al*., 2007; Seki, 2013). The fracture skin layer is also a porous media with low permeability as explained earlier. Therefore, the porosity of the porous fracture skin can also be subjected to such variation due to the diffusion of contaminants into the fracture skin from the fracture and also back diffusion of contaminants from the fracture skin into the fracture. While it is evident that the porosity of the fracture skin can vary based on the above discussion, the variation of the skin porosity with time is a topic yet to be explored. Since the fracture-skin porosity plays a very crucial role in determining the quantum of contaminants that can be removed from the aqueous phase of the fracture, the evaluation of this porosity with time would definitely enable us in characterizing the fate of the contaminants in the subsurface media.

As far as the authors' knowledge is concerned, literature lacks the analysis of contaminant transport mechanism under the influence of time varying fracture skin porosity. The present study is an attempt to analyses the contaminant transport mechanism under time varying fracture skin porosity. The effect of increasing as well as decreasing porosity with time on contaminant transport mechanism is analyzed for four different initial fracture skin porosities of 0.7, 0.1, 0.01, and 0.001. Since there is no established literature on the pattern of porosity variation with time, this study assumes that the skin porosity varies at a particular rate with respect to time. The porosity is assumed to increase at a rate of 1% per day in the present study. Although the rate of variation has been assumed arbitrarily, the purpose of the study is to illustrate the influence of time varying fracture skin porosity on the contaminant transport mechanism in fractured porous media which has not been conducted earlier.

It is very difficult to analyses the effect of time varying fracture-skin porosity through field studies and numerical modeling plays an important role in such situations. In fact, the advantage of numerical modeling is that it can be used to perform studies that are tedious, cumbersome, and sometimes impossible to be conducted in the field. The author feels that this study would provide a breakthrough in understanding the contaminant transport mechanism in complex heterogeneous porous systems where the porosity can vary with respect to time.

2. Physical System and Governing Equations

The conceptual model illustrating a coupled fracture-skin-matrix system (Robsinson *et al*., 1998) is illustrated in Figure 1. A set of parallel fractures having fracture aperture of 2b is separated by a distance of 2H. In between fracture and rock-matrix, the fracture-skin having thickness d-b has been considered. The principal transport mechanisms considered within the fracture include advection, hydrodynamic dispersion, sorption and first-order radioactive decay, and mass transfer to the adjacent skin by diffusion. Molecular diffusion, sorption and radioactive decay have been considered within the fracture-skin and rock-matrix.

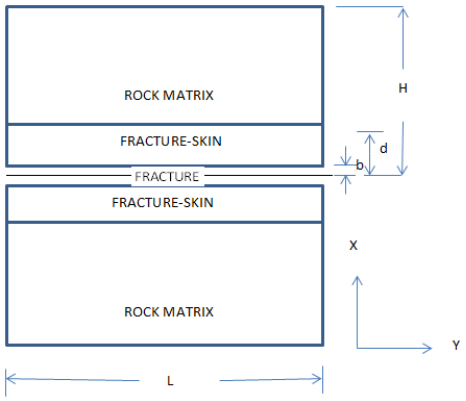


Figure 1. Schematic representation of the coupled fracture-skin-matrix system.

The governing equations for contaminant transport in fracture, fracture-skin and rock-matrix are expressed as (Robinson *et al*., 1998):

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

where $D_L = \alpha_0 V_0 + D^*$ (2)

$$R_s \frac{\partial C_s}{\partial t} = D_s \frac{\partial^2 C_s}{\partial y^2} - \lambda C_s \quad (3)$$

$$R_m \frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial y^2} - \lambda C_m \quad (4)$$

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, x is the space coordinate along the flow direction in the fracture, y is the space coordinate perpendicular to the fracture, t is the time coordinate, D_L is the hydrodynamic dispersion coefficient in the fracture , V_0 is the velocity of the fluid, $\theta_s(t)$ is the time varying fracture skin porosity, D_m is the matrix diffusion coefficient, α_0 is the longitudinal dispersivity in the fracture, D^* is the molecular diffusion coefficient of solute in free water , D_s and D_m are effective diffusion coefficients in fracture-skin and rock-matrix respectively, λ is first order radio-active decay constant. R_f, R_s and R_m are the retardation factors in fracture, fracture-skin and rock-matrix respectively.

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

$$C_f(x,\ t=0)=C_s(x,\ y,\ t=0)=C_m(x,\ y,\ t=0)=0 \quad (5)$$

$$C_f(x=0,\ t)=C_0 \quad (6)$$

$$C_f(x=L_f,\ t)=0 \quad (7)$$

$$C_f(x,\ t)=C_s(x,\ y=b,\ t) \quad (8)$$

$$\theta_s D_s \frac{\partial C_s(x,\ y=d,\ t)}{\partial y}=\theta_m D_m \frac{\partial C_m(x,\ y=d,\ t)}{\partial y} \quad (9)$$

$$C_s(x,\ y=d,\ t)=C_m(x,\ y=d,\ t) \quad (10)$$

$$\frac{\partial C_m(x,\ y=H,\ t)}{\partial y}=0 \quad (11)$$

The following assumptions have been used for modeling coupled fracture-skin-matrix system: 1) Concentrations at the fracture-skin interface, i.e., concentrations along the fracture walls and along the boundary of the fracture-skin are assumed to be equal as expressed in Equation (8). 2) Concentrations at the skin-matrix interface, i.e., concentration along the upper boundary of the fracture-skin and lower boundary of the rock-matrix are assumed to be equal as expressed in Equation (10). The diffusive flux in the fracture-skin is equal to the diffusive flux in the rock-matrix at the skin-matrix interface as expressed in Equation (9). 3) Fracture skin thickness in reality can change with respect to time but for the purpose of simplicity in carrying out the simulations, it is assumed to remain constant with time. 4) As mentioned earlier in the manuscript, there is no established literature on how the fracture skin porosity will vary with respect to time. In this study, fracture skin porosity is assumed to increase or decrease with time at the rate of 1% per day or 10% per day. 5) The minimum porosity of the fracture skin is assumed to not reduce below 0.001 and the maximum porosity is assumed to not increase above 0.9999 as the porosity cannot increase beyond 1 and decrease completely to 0.

3. Numerical Model

The system is described by a set of partial differential equations, one for the fracture, one for the fracture skin, and another for the rock matrix. The coupled non- linear equations are solved using implicit finite difference scheme. The advection part is discretized using upwind scheme and the diffusion part using second order central difference scheme. A varying cell width is adopted in the fracture-skin to capture the flux. Within every time step, first fracture equation is solved, and then the concentration of the fracture is used to solve the governing equations for the fracture-skin. Further, the solution from the fracture-skin is used to solve the rock-matrix equations. Since the methodology for solving these coupled equations has been discussed several times in our earlier work, to avoid repetition the readers are advised to refer them for further understanding (Natarajan & Suresh Kumar, 2010, 2012a, 2012b, 2012c, 2012d, 2014a, 2014b).

4. Results and Discussion

The effect of time varying fracture skin porosity on contaminant transport has been analysed in the present study. The input parameters for the present study have been adopted from Robinson *et al.* (1998). Table 1 shows the parameters used for the validation of the numerical model and Table 2 shows the parameters that were used for the simulation of the present study.

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

Parameters	Value
Average fluid flow velocity in fracture (V_o)	1.0 m/d
Fracture dispersivity (α_o)	$1x10^{-3}$m
Longitudinal Dispersion coefficient within the fracture (D_L)	$1x10^{-3}$ m^2/d
Free molecular diffusion coefficient in water (D*)	$1x10^{-6}$ 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
Length of fracture (L_f)	100 m
Fracture spacing (2H)	0.1 m
Half fracture aperture (b)	$200x10^{-6}$m
Fracture-skin thickness (d-b)	0.002 m
Retardation factor for fracture (R_f)	6
Retardation factor for fracture (R_s)	673
Retardation factor for fracture (R_m)	141
Radioactive decay (λ)	$6.33x10^{-5}$ d^{-1}
Porosity of the fracture skin (θ_s)	0.035

Table 2. Parameters used in the simulation of the present study.

Parameters	Value
Average fluid flow velocity in fracture (V_o)	1.0 m/d
Fracture dispersivity (α_o)	0.1 m
Longitudinal Dispersion coefficient within the fracture (D_L)	0.1 m^2/d
Free molecular diffusion coefficient in water (D*)	$1x10^{-6}$ m^2/d
Effective diffusion coefficient in the rock matrix (Dm)	$4x10^{-6}$ m^2/d
Effective diffusion coefficient in the fracture-skin (Ds)	$4x10^{-6}$ m^2/d
Porosity of rock-matrix (θm)	0.145
Length of fracture (L_f)	25 m
Half fracture aperture (b)	$200x10^{-6}$m
Fracture-skin thickness (d-b)	0.0012 m
Total simulation time	50 days
Retardation factor for fracture (R_f)	6
Retardation factor for fracture (R_s)	673
Retardation factor for fracture (R_m)	141
Radioactive decay (λ)	$6.33x10^{-5}$ d^{-1}

Figure 2a represents the comparison of the results obtained from the present numerical model with the analytical solution provided by Robinson *et al.* (1998). It is observed from Figure 2a that the present model is in close agreement with the analytical solution for contaminant transport in a fracture-matrix coupled system with fracture skin.

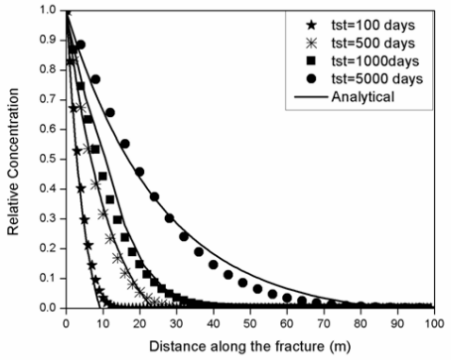


Figure 2a. Comparison of numerical solution with the analytical solution for various simulation time periods for a coupled fracture-skin-matrix system.

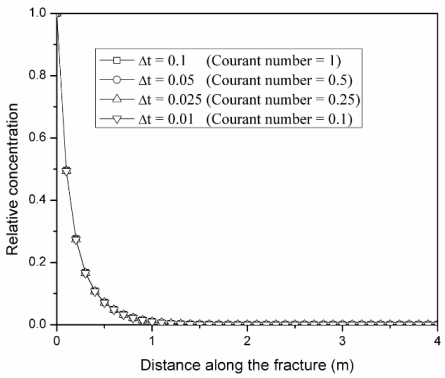


Figure 2b. Relative concentration in the fracture with time varying fracture-skin porosity for different Courant numbers (Porosity increasing at a rate of 1% per day with initial skin porosity of 0.001).

Figure 2b illustrates the spatial distribution of relative concentration in the fracture with time varying fracture-skin porosity (increasing at a rate of 1% per day with initial skin porosity of 0.001) for different Courant numbers. The stability of any numerical model can be determined using the CFL (Courant-Friedrichs-Lewy) condition. The CFL condition is given by the expression

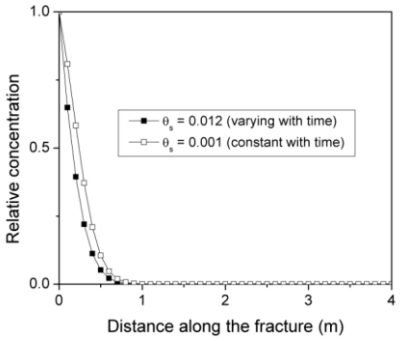
$$Courant \quad number = \frac{velocity * \Delta t}{\Delta x} \tag{12}$$

A numerical scheme is considered to be unconditionally stable if the numerical solution does not possess any oscillation for Courant number ranging from 0 to 1. Since the numerical scheme used in this study is implicit finite difference, the model should be stable even for high Courant number of 1. To ensure the robustness of the numerical model that has been used in this study, the scheme has been tested for different Courant numbers. Space discretization of 0.1m (Δx) was maintained constant while time discretization (Δt) was varied as 0.1, 0.05, 0.025 and 0.01 to yield Courant numbers of 1, 0.5, 0.25, 0.1 using Equation (12). It can be observed from Figure 2b that the concentration profiles do not possess any oscillations irrespective of the Courant number used in the simulation. This shows that the numerical model that was used for the simulation of the concentration profiles for time varying fracture-skin porosity is stable.

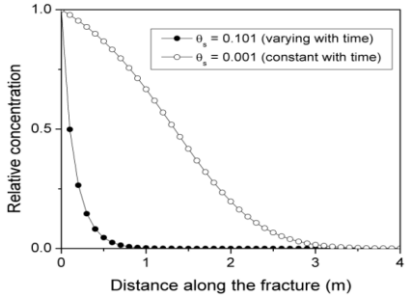
4.1 Fracture skin porosity increasing with time

The fracture skin porosity is assumed to increase at a rate of 1% per day. The effect of this variation on the contaminant transport mechanism is analyzed at the end of 1day, 10 days and 50 days respectively for different initial fracture skin porosities of 0.001, 0.01, 0.1, and 0.7.

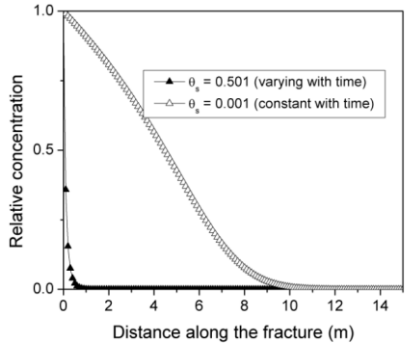
Figure 3 illustrates the spatial distribution of relative concentration of contaminants in the fracture for fracture skin porosity increasing at the rate of 1% per day at the end of 1 day, 10 days and 50 days for an initial fracture skin porosity of 0.001. The contaminant concentration obtained for varying skin porosity has been compared with that obtained using constant skin porosity. The fracture skin porosity at the end of 1, 10 and 50 days are 0.012, 0.101, and 0.501 respectively. It is observed from Figure 3a that the concentration reaches zero within 1m from the fracture inlet at the end of 1 day forboth constant and time varying skin porosity cases. There is a marginal variation in the concentration profile obtained using constant and time varying skin porosity but the profiles reach zero concentration at the same distance from the inlet. It can also be observed that the porosity has increased by an order of magnitude at the end of the 1st day but it does not have a significant impact on the contaminant concentration in the fracture. From figure 3b, at the end of 10 days, the concentration in the fracture reaches zero at a distance of 3m from the inlet for constant skin porosity case but there is a significant reduction in the concentration along the fracture when the skin porosity is increasing. The skin porosity has further increased by an order of magnitude at the end of 10 days. In comparison with figure 3a, it can be noted that for the varying skin porosity case, the reduction in the contaminant concentration in the fracture is not significant at the end of 10 days. The concentration reached zero at 1m from the fracture inletat the end of the 1stday itself as observed from the figure.Thus, when the initial skin porosity is very low (of the order of 0.001)and varying with time, a large quantum of the mass is diffused into the fracture skinwithin a short duration. On the other hand, when the skin porosity remains constant, the diffusion of contaminant mass into the fracture skin reduces with time as observed from the Figures 3a-c. From Figure 3c, it is observed that the fracture skin porosity has risen to 0.501 at the end of 50 days. The contaminant concentration has reached zero at the end of the 1stday when the skin porosity is varying with time but the concentration reaches zero only at 10m from the fracture inlet when the skin porosity is considered constant. Therefore, time varying fracture skin porosity can have a significant impact on the contaminant transport mechanism in the fracture.



(a)



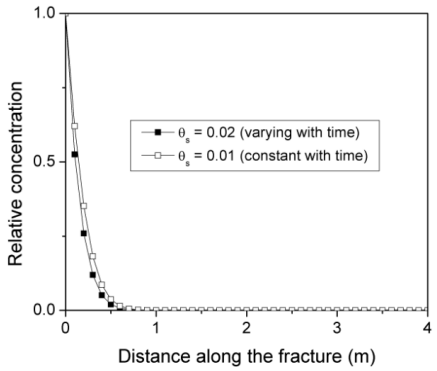
(b)



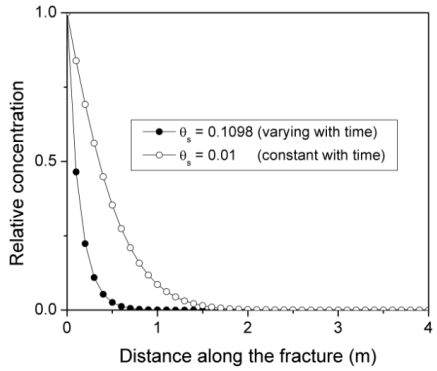
(c)

Figure 3. Spatial distribution of relative concentration along the fracture for increasing fracture skin porosity for initial skin porosity of 0.001 at the end of (a) 1 day (b) 10 days and (c) 50 days.

Figure 4 illustrates the spatial distribution of relative concentration of contaminants in the fracture for fracture skin porosity increasing at the rate of 1% per day at the end of the 1st day, 10 days, and 50 days for an initial fracture skin porosity of 0.01. The contaminant concentration obtained for varying skin porosity has been compared with that obtained using constant skin porosity. The fracture skin porosity at the end of 1, 10 and 50 days are 0.02, 0.1098, and 0.5099 respectively. It is observed from Figure 4a that the concentration reaches zero within 1m from the fracture inlet at the end of 1 day for both constant and time varying skin porosity cases. This is because at the end of the 1st day, the difference is skin porosity for both the cases are negligible. It is observed from Figure 4b that the contaminant concentration reaches zero 2m from the fracture inlet when the skin porosity is constant, while it reaches zero within 1m from the inlet when the skin porosity is varying. The fracture skin porosity has increased by an order of magnitude from 0.01 to 0.1098. In comparison with Figure 4a, the variation of skin porosity from 0.01 to 0.1098 does not have a significant impact on the contaminant concentration in the fracture (concentration reaches zero within 1m from the inlet in Figure 4 a). This observation is similar to that observed for figure 3. From Figure 4c, it is observed that when the initial skin porosity is increased to 0.01 from 0.001, the mass of contaminants diffusing into the fracture skin has increased (concentration reaching zero 3m from the inlet) compared to the observation in Figure 3c.



(a)



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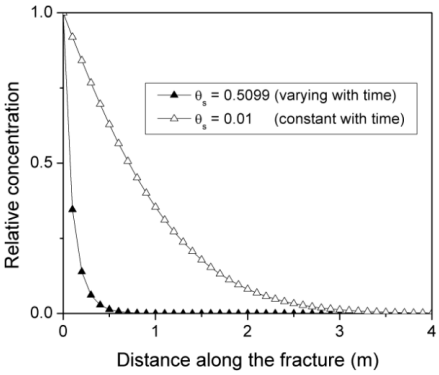

(c)

Figure 4. Spatial distribution of relative concentration along the fracture for increasing fracture skin porosity for initial skin porosity of 0.01 at the end of (a) 1 day (b) 10 days and (c) 50 days.

Figure 5 illustrates the spatial distribution of relative concentration of contaminants in the fracture for fracture skin porosity increasing at the rate of 1% per day at the end of the 1st day, 10 days and 50 days for an initial fracture skin porosity of 0.1. The contaminant concentration obtained for varying skin porosity has been compared with that obtained using constant skin porosity. The fracture skin porosity at the end of 1, 10, and 50 days are 0.1099, 0.1998, and 0.5999 respectively. It is observed from Figure 4a there is no variation in the concentration profile obtained from both the cases. This is because the skin porosity variation at the end of 1 day is negligible and does not influence the contaminant concentration. It is observed from Figure 5b that the variation in the concentration profiles of both cases is not considerable.

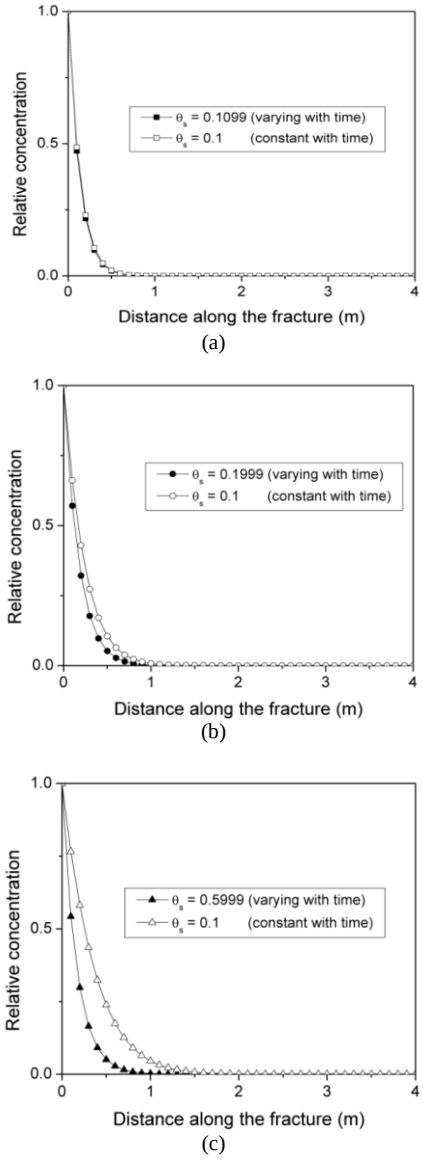

Figure 5. Spatial distribution of relative concentration along the fracture for increasing fracture skin porosity for initial skin porosity of 0.1 at the end of (a) 1 day (b) 10 days and (c) 50 days.

There is a marginal variation in the contaminant concentration obtained using constant and varying skin porosity at the end of 50 days as the skin porosity has marginally increased from 0.1 to 0.5999. It can be observed from Figures 5a-c that the concentration reaches zero within 2m from the inlet at the end of 1, 10, and 50 days when the skin porosity is maintained constant. Therefore, progressively increasing diffusion of contaminant mass takes place from the fracture to the fracture skin when the constant fracture skin porosity is increased by orders of magnitude as observed from Figures 3c, 4c, and 5c.

Figure 6 illustrates the spatial distribution of relative concentration of contaminants in the fracture for fracture skin porosity increasing at the rate of 1% per day at the end of the 1stday, 10 days, and 50 days for an initial fracture skin porosity of 0.7. The contaminant concentration obtained for varying skin porosity has been compared with that obtained using constant skin porosity.

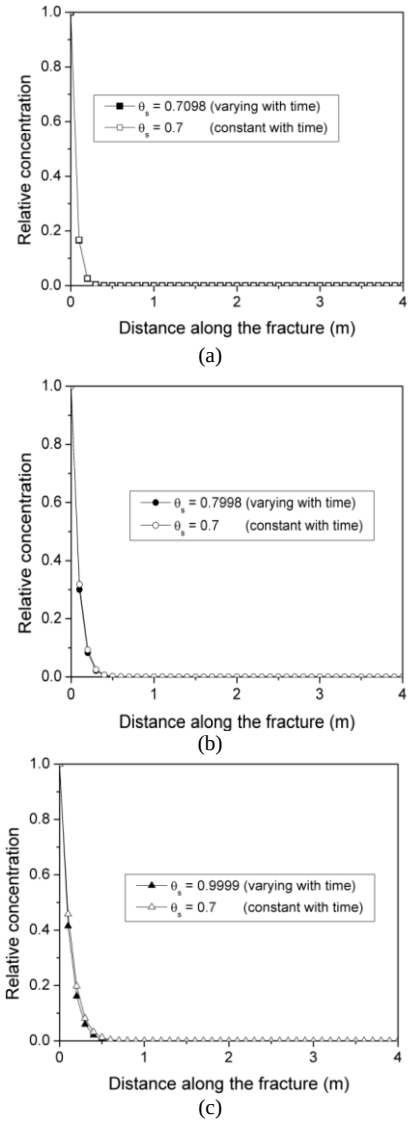

Figure 6. Spatial distribution of relative concentration along the fracture for increasing fracture skin porosity for initial skin porosity of 0.7 at the end of (a) 1 day (b) 10 days and (c) 50 days.

The fracture skin porosity at the end of 1, 10, and 50 days are 0.7098, 0.7998, and 0.9999 respectively. It is observed from Figure 6a-c that there is no difference between the profiles obtained using constant skin porosity and time varying skin porosity. This is because the fracture skin porosity of 0.7 is so large that varying the fracture skin porosity with time beyond 0.7 does not have any impact on the contaminant concentration in the fracture. Therefore, time varying fracture skin porosity does not have any effect when the initial fracture skin porosity is very large.

Figure 7 illustrates the spatial distribution of relative concentration of contaminants in the fracture for various fracture-skin diffusion coefficients with porosity increasing at the rate of 1% per day. It is observed from the figure that similar to the constant skin porosity case, the solute concentration in the fracture is very low when the fracture-skin diffusion coefficient is very high (D_s = 4 e-06 m^2/d). The solute concentration increases with decrement of the skin diffusion coefficient. Moreover, since the porosity is increasing within the fracture-skin with time, the concentration in the fracture is rapidly decreasing and thus concentration becomes zero within 6m from the fracture inlet in all the cases considered.

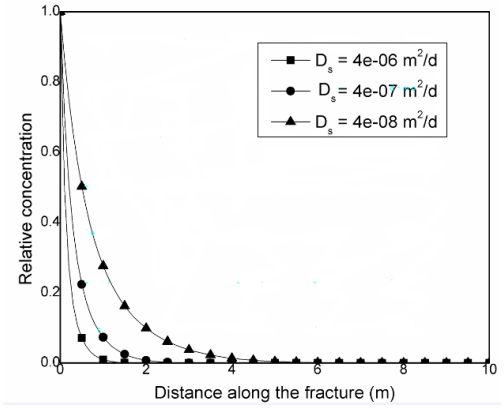

Figure 7. Spatial distribution of relative concentration of contaminants in the fracture for various fracture-skin diffusion coefficients with porosity increasing at the rate of 1% per day (initial porosity = 0.001).

Figure 8 illustrates the spatial distribution of relative concentration of contaminants in the fracture for various half fracture apertures with porosity increasing at the rate of 1% per day. It is observed from the figure that the solute concentration is high in the fracture for very high half fracture aperture (b = 500e^{-06}m) and the solute concentration reduces with decrement of the fracture aperture. This is because the coupling between the fracture and the fracture-skin becomes stronger with the reduction of the half fracture aperture. The time varying fracture-skin porosity causes rapid diffusion of contaminants into the fracture-skin and consequently the concentration reduces to zero very close to the inlet of the fracture.

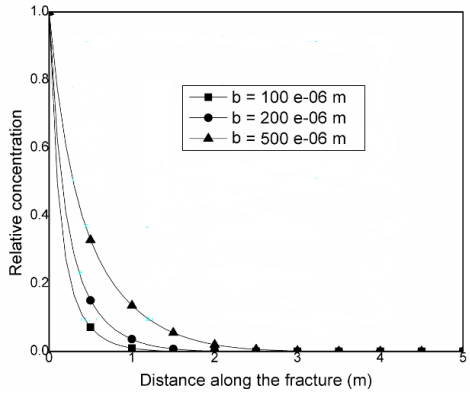

Figure 8. Spatial distribution of relative concentration of contaminants in the fracture for various half fracture apertures with porosity increasing at the rate of 1% per day (initial porosity = 0.001).

5. Conclusions

A numerical model is developed to analyze the effect of time varying fracture skin porosity on the contaminant transport mechanism in fractured porous media. The set of coupled equations for contaminant transport is solved using implicit finite difference method. Constant continuous source of contaminants is assumed at the inlet of the fracture. The flux transfer at the interface of the fracture and the fracture skin is captured by adopting a varying grid pattern. The fracture skin thickness is assumed to be constant during the simulation time but the fracture skin porosity is assumed to vary with time. The effect of increasing fracture-skin porosity with time on the contaminant transport mechanism has been analyzed for various initial fracture skin porosities. The following conclusions have been made based on the above study: 1) Large quantum of contaminant mass diffuses from the fracture into the fracture skin within a short duration when the initial fracture skin porosity is very low and increasing with time. 2) The effect on the contaminant transport mechanism is negligible when the initial fracture skin porosity is high and increasing with time. 3) The concentration rapidly reduces within the fracture for various half fracture apertures and fracture-skin diffusion coefficients due to the effect of time varying fracture-skin porosity.

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