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Probabilistic analysis of contaminant transport in fractured sedimentary rocks

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ABSTRACT

Understanding the flow and contaminant transport process in rocks has received increased attention in the past two decades as these geological formations serve as potential sites to contain different types of wastes in geological repositories. In this paper, a discrete fracture network model is developed to understand the process of contaminant transport in a fractured rock mass. This model integrates a stochastic fracture generating algorithm for sedimentary rocks and a two-dimensional numerical model that simulates the flow and transport of a contaminant through the heterogeneous system of fractures. Further, the uncertainty in geological and transport properties of the contaminant are considered as random variables. The probability of concentration exceeding the permissible value at the endpoint is quantified by carrying out reliability analysis using the subset simulation method. The probabilistic framework developed in this study helps assess the behaviour of contaminant migrating through a complex heterogeneous system and provides a basis for gaining a level of confidence in the model results.

Keywords: sedimentary rocks, discrete fracture network model, fracture generation algorithm, random variables, reliability analysis, contaminant transport

1 INTRODUCTION

In designing waste disposal systems such as landfills (or radioactive waste repositories), there are numerous problems of environmental concern which involve migration of contaminant plumes due to their leakage from the disposal systems. So, the fundamental design objective of a disposal system is to ensure its long-term safety. Since the safety is sought over large spatial and temporal scales, the variations in the surrounding geosphere will have a potential impact on the overall performance of these systems. So, it becomes imperative to model the geological environment in order to predict the movement of contaminant through the geosphere, especially when the disposal systems are designed near rocky subsurface formations. However, modelling a rock mass is quite challenging due to the presence of ubiquitous natural discontinuities known as fractures. Flow and transport through individual fractures, as well as fracture networks, has been studied over the past five decades. Many analytical models have been developed to describe the flow and transport of contaminant through fractured rock (Bear et al., 1993; NRC, 1996; Neuman, 2005). Further, the geometrical complexities in the medium were handled by developing numerical models. Freeze and Cherry (1979) drew attention to the importance of matrix diffusion involving discrete fractures in contaminant hydrogeology for fractured porous media, including sedimentary rock and fractured clayey deposits. Further, the need to consider fractures exclusively was emphasized, confirming the significance of fracture geometry on the hydrological behaviour of the rocks (Long et al., 1989). This led to the development of discrete fracture network (DFN) models, where each fracture is explicitly represented by its geometry (by their orientation, size, aperture etc.), and the relation between fractures and fracture sets are also described. Many studies adopted the DFN approach for contaminant transport modelling in fractured rock (Smith and Schwartz, 1984; Alexander et al., 2003; Parker et al., 2012; Lei et. al., 2017). However, most of these works have been limited to modelling the flow and transport of contaminant in a fractured medium deterministically. Assuming the geological and transport properties in the medium to be constant leads to unrealistic modelling. So, there is a need to account for the uncertainties involved in the system to assess the long-term safety of waste disposal systems. Very few studies have considered the stochasticity in the geohydrological properties of the fractures and intact rock and; transport properties of the contaminant (reactive and non-reactive) to understand their influence on the concentration plumes as they can lead to subsurface contamination (Toran et al., 1995; Nair and Krishnamoorthy, 1999; Piscopo et al., 2017). But, characterizing and quantifying the effect of uncertainties in fractured medium on contaminant transport process has received comparatively less attention in the literature. So, in this paper, a

probabilistic framework has been developed to predict the behaviour of contaminant through a complex heterogeneous system of fractures and quantify the effect of uncertainties on the concentration pattern of contaminant using effective probabilistic techniques

2 GEOSPHERE TRANSPORT MODEL

The two primary components involved in modelling contaminant transport in fractured rock are:
1. Geometric representation of fracture pattern by means of discrete fracture network model.
2. Development of a numerical model that solves the flow and transport process along fractures and intact rock matrix.

2.1 Algorithm for fracture generation

The flow and transport of contaminant in the fractured rock mass is governed by a heterogeneous system of fractures. So, it is necessary to simulate the natural fracture network explicitly with respect to their geometry. In this study, the fracture patterns have been generated based on the stochastic fracture generation algorithm developed by Riley (2004). This algorithm essentially generates the fracture trace length distributions and fracture spacing distributions are derived for a given fracture density and orientation distribution of layered rocks. For a given fracture set, the algorithm is a function of fracture density, fracture orientation, the velocity of crack propagation and the probability with which the fracture terminates. A typical fracture pattern generated from the algorithm is presented in Fig. 1.
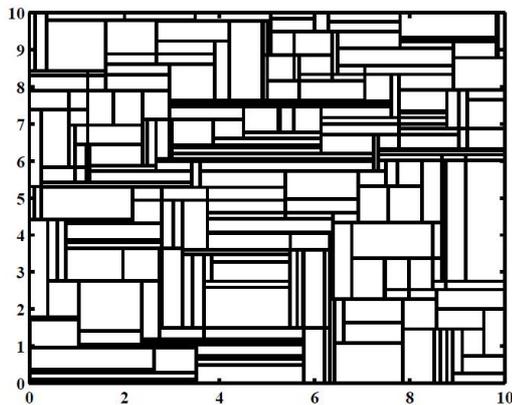

Fig. 1. Fracture patterns generated for 0°-90° set using the algorithm.

2.2 Numerical Model

The contaminant transport is modelled using Finite Element and subsurface FLOW systems (FEFLOW). FEFLOW is numerical modelling software developed by Hans-Jorg. G. Diersch (Diersch, 2014) to model groundwater flow and contaminant transport problems in porous and fractured media. A two-dimensional finite element model with a fractured network generated based on the DFN concept is developed. The porous

media and the set of fractures are represented as two distinct interacting subsystems coupled through interfaces and the contributions from both these subsystems are assembled to compute the concentration through the medium. The finite element mesh generated for a fractured rock mass is presented in Fig. 2.
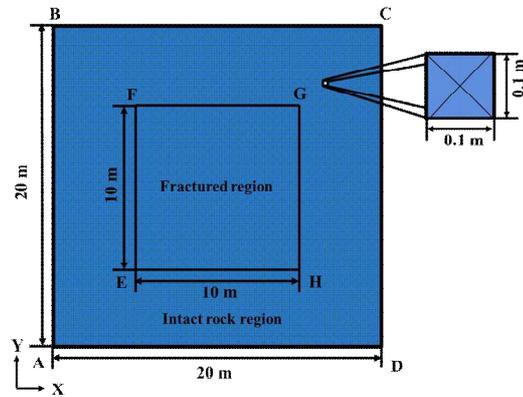

Fig. 2. Fracture patterns generated for 0°-90° set using the algorithm.

2.3 Aperture variation along the fracture

An additional component that considers the variation in aperture sizes along fracture is also modelled. The local parallel plate concept of approximation has been used to simulate local aperture variations along the fracture. Each fracture is divided as a series of 'n_p' discrete segments with different aperture sizes. The number of segments in each fracture is a function of the length of each element in finite element mesh, the length of fracture and the extent of variations observed from in-situ/experimental investigations. By integrating the effect of all these factors, the maximum number of segments in a fracture is given by

$$n_p = l_f / l_e \qquad (1)$$

where n_p, l_f and l_e are the maximum number segments in each fracture, length of the fracture and the length of the element in the finite element mesh, respectively. A schematic of variation in aperture sizes along the fracture is presented in Fig. 3.

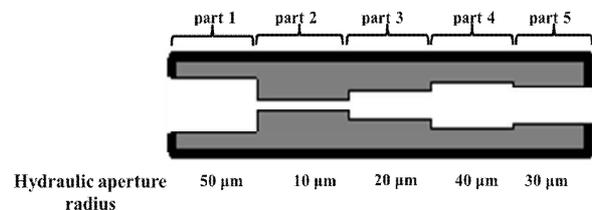Fig. 3. Schematic of aperture variation along the fracture

2.4 Python programming interface

The three components of the DFN model which include (1) generation of fractures using a stochastic algorithm, (2) generation of finite element mesh that

models the fluid flow and contaminant transport process in fractures and intact rock matrix and, (3) generation of aperture variation along the fracture are integrated using the python programming interface.

3 INPUT PROPERTIES CONSIDERED FOR THE STUDY

In this study, the flow and transport behaviour of non-reactive contaminant in a complex fracture sedimentary rock is investigated. The geohydrological parameters of the medium and contaminant transport properties are presented in Table 1.

Table 1. Geological properties of rock (Diersch, 2014).

Quantity	Value
Study Domain	
Length (m)	20
Width (m)	20
Porous matrix	
Isotropic hydraulic conductivity (m/s)	10^{-9}
Porosity	0.13
Molecular diffusion(m^2/s)	5×10^{-10}
Longitudinal dispersivity (m)	1
Transverse dispersivity (m)	0.5
Fracture	
Fracture area (m^2)	6×10^{-5}
Hydraulic aperture (m)	1.2×10^{-4}
Hydraulic radius (m)	6×10^{-5}
Longitudinal dispersivity (m)	0.1
Molecular diffusion (m)	5×10^{-9}

From the previous studies, it could be noted that the general range of fracture orientations observed from the field and modelling investigations was 0°-130° (Bai and Pollard, 2000; Burg, 2012; Yue et al., 2017). The most frequently occurring fracture patterns are horizontal and vertical fractures. So, fracture orientations considered for the study are 0° and 90°. The other input parameters of the fracture generation algorithm are presented in Table 2.

Table 2. Input properties for fracture generation.

Quantity	Value
Length of fracture domain in x-direction (m)	10
Length of fracture domain in y-direction (m)	10
Number of fracture sets	2
Density of fractures	1, 2
Inhibition distance	0.1
Probability of continuation after fracture intersection	0.1

A rock mass of size 20 m × 20 m is considered (ABCD in Fig 2) and a network of fracture of dimension 10 m × 10 m (EFGH in Fig 2) is modelled within the domain. This domain is discretized into a two-dimensional quadrilateral mesh with 40401 nodes and the fractures are modelled as 1D discrete elements. Each quadrilateral element is refined further into four small triangular elements leading to 80401 nodes in the mesh and presented in Fig. 2. Further, the flow and transport

boundary conditions are assigned to the domain and presented in Table 3 (notations in Fig. 2).

Table 3. Boundary conditions of the domain.

Section	Quantity	Value
Fluid flow		
AB	Dirichlet-type (-5≤y≤15, x = -5) (m)	10
DC	Dirichlet-type (-5≤y≤15, x = 15) (m)	20
Mass transport		
IJ	Dirichlet-type (0≤y≤10, x = -5 m) (mg/l)	1
AI	Dirichlet-type (-5≤y≤0, x = -5 m) (mg/l)	0
IB	Dirichlet-type (0≤y≤15, x = -5 m) (mg/l)	0

Further, to demonstrate the influence of variation in aperture size along the fracture, a parametric study is carried out. Here, the number of segments (m) within each fracture is varied from one (segment) to five (segments). The typical range of aperture values considered in the literature (1 × 10^{-5} m to 5 × 10^{-5} m) has been used (Wendland and Himmelsbach, 2002; Graf and Therrien, 2005). A random combination of aperture sizes is considered for the analysis and presented in Table 4.

Table 4. Hydraulic aperture sizes considered in the study.

Number of parts	Value
One (m)	5×10^{-5}
Two (m)	5×10^{-5}, 1×10^{-5}
Three (m)	5×10^{-5}, 1×10^{-5}, 2×10^{-5}
Four (m)	5×10^{-5}, 1×10^{-5}, 2×10^{-5}, 4×10^{-5}
Five (m)	5×10^{-5}, 1×10^{-5}, 2×10^{-5}, 4×10^{-5}, 3×10^{-5}

4 PROBABILISTIC ANALYSIS

There is a need to account for uncertainties in the geological and transport properties of the medium and contaminant that could have a great impact on the prediction of contaminant concentration. So, these properties are modelled as random variables to account for randomness in fracture generation. The mean values (underlying normal distribution) of the input parameters, the probabilistic distribution and coefficient of variation (COV) have been assumed from literature and shown in Table 2 (Riley, 2004; Aladejare and Wang 2017). The influence of these uncertainties on the system is quantified by estimate the probability of concentration exceeding its permissible limit by employing efficient probabilistic techniques. So, the probability of concentration exceeding its permissible value is estimated from the equations

$$P_f = P[g(x) < 0] \qquad (2)$$

$$g(x) = C_0 - \max[C(X,t)] \qquad (3)$$

where $X - [X_1, X_2 \cdots X_9]$ is the vector of random variables, $g(x)$ is the limit state function, C_0 is permissible concentration and, $C(X,t)$ is the maximum

concentration within the time period t computed from the numerical model.

Table 5. Statistical properties of the random variables.

Property	Iodine Mean	Iodine COV	Distribution
Rock matrix			
Hydraulic conductivity (m/s)	10^{-4}	0.40	Lognormal
Porosity	0.13	0.40	Lognormal
Fracture			
Fracture aperture, part 1 (μm)	50	0.40	Lognormal
Fracture aperture, part 2 (μm)	10	0.40	Lognormal
Fracture aperture, part 3 (μm)	20	0.40	Lognormal
Fracture aperture, part 4 (μm)	40	0.40	Lognormal
Fracture aperture, part 5 (μm)	30	0.40	Lognormal
Diffusion coefficient (m²/s)	5×10^{-9}	0.40	Lognormal
Longitudinal dispersivity (m)	0.1	0.40	Lognormal

4.1 Subset simulation

Estimating the probability of failure of a rare event is challenging as they have very small failure probabilities. It becomes unreliable to opt for conventional techniques like Monte Carlo simulation, FORM / SORM etc as they not only become computationally demanding but also leads to questionable results in achieving a convergence towards the actual solution. An alternative and efficient technique called subset simulation is developed to estimate the P_f for such rare events (Au and Beck, 2001). The underlying idea in subset simulation is to break down a rare event into a sequence of frequently occurring events. Let the failure event denoted as F be a sequence of intermediate events such that $F_1 \supset F_2 \supset \cdots F_n = F$. Thus, the failure event is nothing but the intersection of all the intermediate events. By conditioning the event F_i sequentially, the failure probability P_f is

$$P_f = P(F_1) \prod_{i=1}^{n} P(F_{i+1} | F_i) \qquad (4)$$

For the simulation 1000 samples are consider per subset and the conditional probability is constantly maintained as $P(F_1) = 0.1$. A python program is written, and subset simulation runs are automated.

5 RESULTS AND DISCUSSION

The inventory of contaminant released from the system is estimated. Since, the contaminant is non-reactive, the contaminant concentration released from the system has a relative concentration of $C/C_0 = 1$, where C is the concentration at time t and C_0 is the initial concentration. The three modules of the geosphere transport model are integrated to develop a finite element mesh with fractures (as in Fig. 1) and variations in aperture size along the fractures (as in Fig. 3). The input properties of fracture and intact rock

matrix are assigned to the model and the extent of influence a set of fractures can create on the contaminant transport is investigated. The spatial extent of fracture network and their heterogeneity makes it difficult to predict the pathway of contaminant movement through the system. So, some critical observation points are considered as shown in Fig. 4. The evolution of contaminant concentrations over time are evaluated at these points.
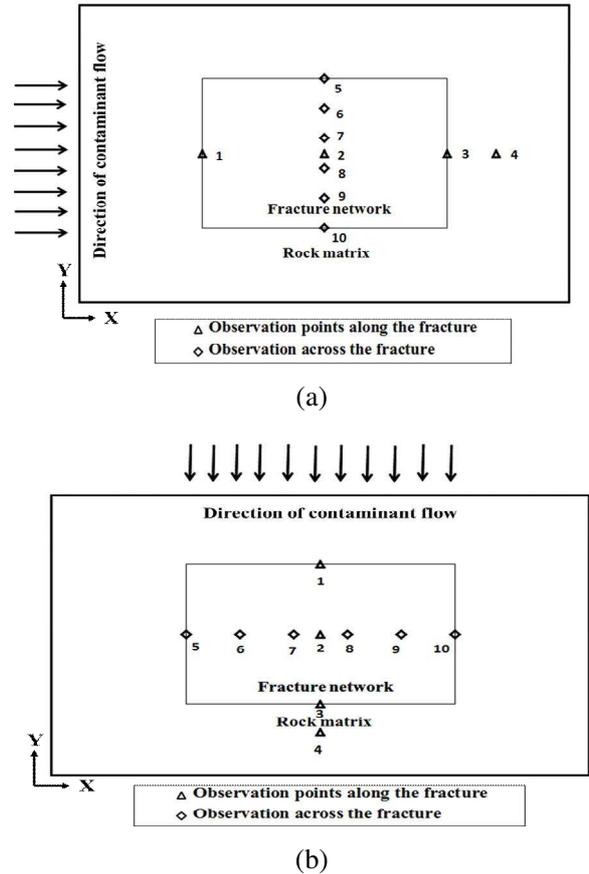

(a)

(b)

Fig. 4. Observation points when the contaminant flow is (a) along x-direction (b) along y-direction

Fig. 5 presents the results of concentration trends observed at different points when the contaminant travelled through the 0°- 90° fracture set. Among the 200 fractures generated from the fracture generation model, 100 of them are oriented at 0° and 100 of them at 90°. Fig 5(i) and 5(ii) present the cases when the contaminant flow is along x and y directions, respectively. From these plots, it can be observed that the contaminant is spread out along and across the domain. But to understand the extent of heterogeneity in the system, Fig. 5(iii) and Fig. 5(iv) are plotted. In Fig. 5(iii), the results for observation points orthogonal to the flow direction are plotted (i.e., blue trend lines for observation points 5(a) - 10(a); red trend lines are for observation points 5(b) - 10(b)). These observation points are orthogonal to the flow direction.

(i)   Concentration versus for flow along x- direction

(ii) Concentration versus time for flow along y- direction

(iii) Concentration versus time at points transverse to flow direction

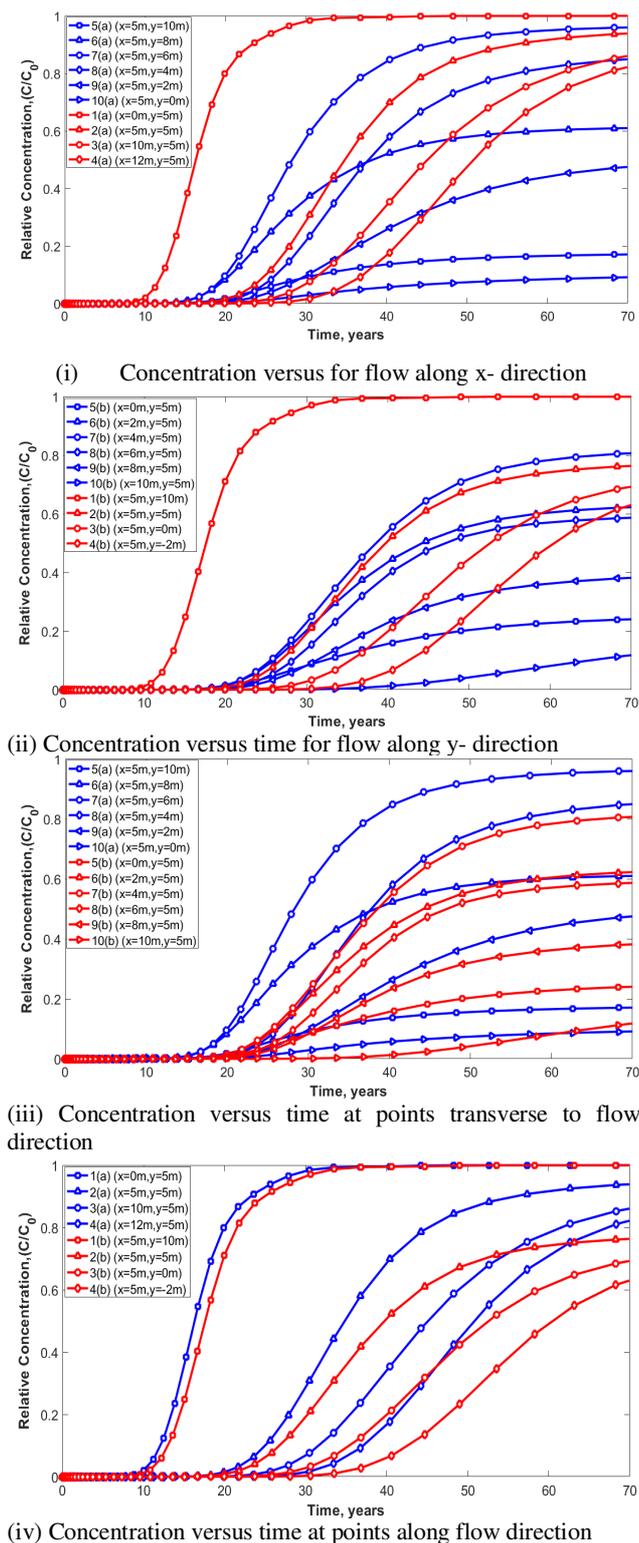(iv) Concentration versus time at points along flow direction

Fig. 5. Concentration versus time for different cases of 0°- 90° fracture set

From the results, it is evident that there is heterogeneity in the system and the time take for the arrival of maximum concentration is faster when the flow of contaminant is in the x-direction. Similarly, Fig. 5(iv) presents the results for observation points along to the flow direction (i.e., blue trend lines for observation

points 1(a) - 4(a); red trend lines are for observation points 1(b) - 4(b)). This plot also demonstrates the difference in the concentration values from both the cases. The influence of heterogeneity in the fracture network and variation in concentration plumes for flow along x and y directions are presented from this analysis. The endpoint of assessment is 10 m from the source and the time of arrival of maximum concentration (i.e., $0.8C_0$) at this point is at around 70 years. Further, a parametric study is carried out to demonstrate the influence of aperture variations along the fracture. The aperture size combinations presented in Table 3 were considered for the analysis to generate the fracture network. The concentration trends at three observation points (represented in blue (point 2(a)), green (point 4(a)) and red (point 10(a))) and for five aperture variation combinations (represented in different markers) are presented Fig. 6. The results show that there is a significant effect of this factor on the contaminant concentration values. The results do not follow a definite trend with respect to increasing aperture size variations
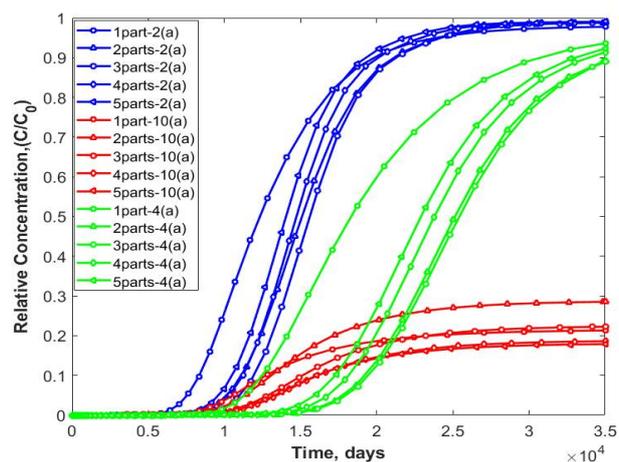

Fig. 6. Concentration trends for different cases of aperture variations along the fracture - Horizontal flow direction

However, the concentration values are affected by at least 0.2% to almost 20% of their initial value due to local variation in aperture size.

The results from the deterministic analysis showed that the concentration of the contaminant at the endpoint of interest was less than the permissible value (i.e., $C_0 = 1$ mg/l). By running the automated python programming module, which has the subset simulation algorithm, P_f is estimated. The probability of the concentration of contaminant exceeding its permissible value (P_f) is 4.6×10^{-4}. This value indicates that, for the time scale considered for the study and under the influence uncertainties in the geological and transport properties of the model, the possibility of contamination is very low, suggesting that the possibility of contamination is very low at the endpoint.

6 CONCLUSIONS

A numerical model is developed to describe the flow and transport of a contaminant in a fractured rock mass. This model simulates the fracture patterns from a stochastic algorithm, models the flow and transport of contaminant and, quantifies the contaminant migration through the system. It also captures the features of fracture geometry, variation in aperture sizes along the fracture and their influence on contaminant migration. To illustrate the contaminant flow process using the model, a 0°- 90° fracture set combination is considered for the analysis. The contaminant concentrations are evaluated at different points spread along and across the domain to understand contaminant spread in the entire fracture network. The results showed that there is an influence of heterogeneity in the fracture network. There are preferential flow paths that lead to channeling of contaminants and presence of a complex fracture network results in slower movement of contaminant. The deterministic analysis results showed that the concentration at the endpoint (i.e., 10 m from the source) is always less than the peak concentration, which implies that it is within safe limits. Also, due to local variation in aperture sizes, the concentration value is affected at least by 0.2% to almost 20% of its initial value, indicating that the arrangement of aperture variations along the fracture plays an important role in predicting the concentration of the contaminant. Further, the uncertainty in the geological and transport properties of the medium and the contaminant were considered. Their effect was quantified using the subset simulation method. The deterministic and probabilistic components of the model are integrated through a python programming interface which helped in making the model computationally efficient. The P_f value estimated from the model was very low. Thus, the reliability analysis results quantify the extent of pollution possible due to contaminant migration under the influence of various uncertainties through any fracture network.

ACKNOWLEDGEMENTS

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