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RESEARCH PAPER

NUMERICAL MODELING OF CONTAMINANT TRANSPORT IN FRACTURED CRYSTALLINE ROCKS (FCRS) OF THE ACCRA-TEMA AREA, SOUTHEASTERN GHANA

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ABSTRACT
The prediction of contaminant transport in saturated fractured media is a difficult task, due to the complexity of fracture geometry, connectivity, heterogeneity and anisotropy of hydraulic conductivities and chemical processes. Generally, the simulation of contaminant transport in fractured media is by the discrete fracture network (DFN) approach. However, this approach is not appropriate for district to regional scale due to computational challenges and the extensive data required by discrete fracture models for fracture system characterisation. In this paper, a hybrid approach that combined the advective-dispersion equation (ADE) continuum model, and discrete fracture network (DFN) simulation is used for the prediction of the contaminant transport in the fractured crystalline rocks within southeast Ghana. The hydrogeology of the study area consists of crystalline rocks with negligible matrix porosity. The approximate geometry of the problem was represented as a horizontal aquifer without curvature, and no-flow boundaries existing at the top and bottom of the aquifer. A MATLAB code is developed for the finite difference method to obtain the numerical solution. The study demonstrates that, the major factors affecting contaminant migration in the study area include, hydraulic conductivity which depends on fracture connectivity, aperture and infill material, and the retardation factors of the various contaminants. Results of transport simulation indicate that, contaminants could travel between 1.0 to 1.7 m/day in the horizontal direction. This spreading effect of plume movement through the fractured rocks can pose critical environmental problems.

Keywords: *Contaminant transport, numerical modelling, fractured media, two-dimension, finite difference method*

INTRODUCTION
Groundwater is found in rocks in the subsurface in most areas, at relatively shallow depths. It represents about two-thirds (2/3) of global water (Fetter, 1998). It moves at varying velocities ranging from metre per millennia to metre per day (Konikow and Glynn, 2005). Flowing groundwater is a major mechanism or the

transport of chemicals, and a major pathway from rocks to human exposure and consumption. Groundwater provides about 45% of the public water supply in Ghana (Adomako *et al*., 2011). Most of the rural population in the country, supply their own drinking water from domestic dugout wells and pumps. Consequently, groundwater is considered an important source of portable water in every part of the country. The main concern of groundwater is quality and pollution (Musolff, 2009).

The prediction of contaminant transport in saturated fractured media is not an easy task, due to the complexity of fracture geometry and connectivity, heterogeneity and anisotropy of hydraulic conductivities, and the chemical processes involved (Freeze and Cherry, 1979; Domenico and Schwartz, 1990).

The flow of groundwater and transport of contaminants depends on the hydraulic conductivity and hydraulic gradient of the particular aquifer, which in turn depends on whether the aquifer has an intergranular or fracture permeability. Flow velocity and contaminant migration can be several times higher in the case of fracture permeability (Christopher and Leslie, 1994), compared to the case of intergranular permeability. The motivation of this study is from conditions of the study area, the Accra-Tema area (ATA) in southeast Ghana (Fig. 1). The area is underlain by two major rock formations, the Togo Structural Units (TSU) and the Dahomeyan Gneissic Complex (DGC).

The rocks in these areas are crystalline in nature that is, they are hard consolidated rocks, and assumed to have no primary porosity (Kesse, 1985). The means of storage and flow of groundwater, is by the presence of fractures (Darko, 2001). The area is within a regional highly deformed tectonic zone, referred to as the Pan-African Mobile belt (Affaton *et al*., 1991). The rocks are intensely fractured (Kesse, 1985; Tairou *et al*., 2012). Most of the inhabit-

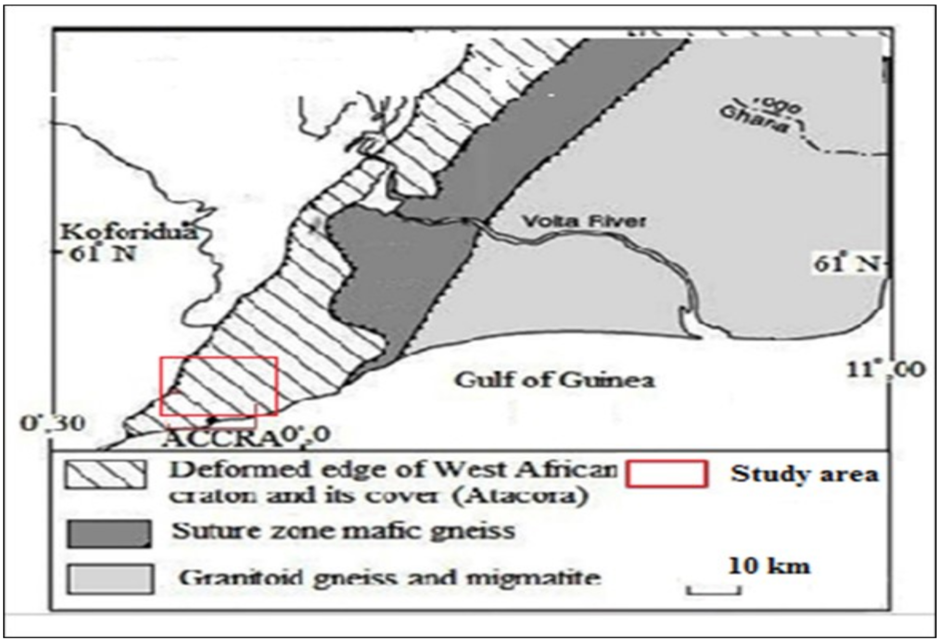

Fig. 1 Tectonic map of SE Ghana, showing the study area (Modified after Attoh, 1998)

ants in the study area (urban and peri-urban) are heavily dependent on groundwater for their source of potable water, agricultural, and other domestic use. Despite the importance of groundwater resource in Ghana, little attention has been paid to exploring measures that can help reduce activities that have the high potential of adversely impacting on the quality of groundwater. It is important to find measures to prevent the high potential of groundwater pollution and probably declining trend of groundwater quality.

Mathematical models are commonly used in the management of groundwater resources, particularly as a tool to predict contaminant transport (Elsworth, 1987), extent of contamination, evaluation of dense non-aqueous phase liquids (DNAPL) source zone longevity, and cost/benefit of a selected remediation technology (Khebchareon and Saenton, 2005).

Modelling groundwater flow in fractured rocks is comparatively more complex compared to modelling in the case of porous rocks. This is because, fractures are not only difficult to observe and characterise, but also difficult to represent in a numerical model. Based on the present state of understanding of flow and contaminant transport mechanism, flow and transport problems in fractured media can be described using mathematical models (Freeze and Cherry, 1979). The descriptions are made using a system of partial differential equations or governing models together with initial and boundary conditions.

In order to solve a given flow problem, the system of equations must be solved for the specific data of the problem. This can be done using either analytical or numerical techniques. However, for most problems of practical interest, due to the irregular shapes of most of the boundaries, the spatial variability of the coefficients appearing in the equations and in the boundary conditions, the non-uniformity of the initial conditions, and the non-analytic form of the various source and sink terms, analytical solutions are mostly not possible, except for relatively simple problems. Solution of most problems are thus often obtained by numerical methods (Konikow and Glynn, 2005). In the present investigation, an attempt was made to provide a simple but sufficiently accurate methodology for numerical simulation of the two-dimensional contaminant transport through the saturated heterogeneous media using finite difference approach. Finite difference method (FDM) has been adopted to solve the one dimensional contaminant transport equation to predict the pollutant migration through the fractured crystalline rocks (FCR). In the use of this approach, the velocity field is first determined within a hydrologic system, and these velocities are then used to calculate the rate of contaminant migration by solving the governing equation.

Discrete fracture network (DFN) models provide a more flexible alternative approach in this situation (Derschowitz *et al*., 1998). However, the DFN models are computationally intensive and are not feasible, due to computational limitations, for applications involving large rock volumes (Dverstrop *et al.,* 1992).

In this study, a hybrid approach (NRC, 1996) that combines the ADE continuum model with DFN simulations was explored. The 'very far' concept of up-scaling proposed by Bear and Berkowitz (1987) was adopted.

A MATLAB code was developed for the finite difference method to obtain the numerical solution.

The code was used to predict heavy metal transport using lead (Pb) as the surrogate. This was chosen as an example when dealing with heavy metals that are persistent (Prommer *et al.,* 2002). The initial concentration of Pb was based on the assumption of a constant leakage of 100 mg/L leachate of mixed municipal waste dump into the fractured rock aquifer.

The finite difference technique is well suited for complex geometries, complicated flow patterns, heterogeneity, and nonlinearity (Rowe 1988). In this study, a two-dimensional (2-D) domain, splitting into regular rectangular grids or meshes of width k in the time *t*- direction and depth *h* in the space z-direction, is simulated for 2-D contaminant transport. It describes concentration of the contaminant species at different times.

Mathematical model for flow and contaminant transport in fractured media

Studies in groundwater flow and contaminant transport have been carried out in porous media, including soils (Cacas *et al*., 1990), porous fractured (Van Golf-Racht, 1982) and fractured media (Lomize, 1951; Rommin, 1966; Nelson, 1985) and various models have been advanced (Anderson and Woessner, 1992). However, only a few of the investigators have derived the basic equations describing fluid flow and contaminant transport through fractured rocks.

According to Bear (1993), there are three main approaches to modelling of fracture flow: (1) equivalent porous medium models, used for large-scale problems if there is no need for knowing the flow field in detail, (2) double porosity models which work with two connected continua, representing fractures and porous blocks, and (3) stochastic discrete fracture network (SDFN) models which try to create an approximate representation of the fractured environment as possible by simulating particular fractures. Due to computational costs SDFN models are normally used for solution of the problems on relatively small domains (up to tens of metres) (Reeves *et al*, 2008). The approach adopted in this study is based on SDFN model. Here, a hydrodynamic model based on a set of coupled differential equations are developed.

A general form of the governing equation which describes the 3-D movement of groundwater with constant density through porous media is (Freeze and Cherry, 1979):

$$\frac{\partial}{\partial x_i}\left(K_i \frac{\partial h}{\partial x_i}\right) - q_s = S_s \frac{\partial h}{\partial t} \qquad (1)$$

where, K_i is the saturated hydraulic conductivity tensor (LT^{-1}), q_s is the volumetric flux of water per unit volume, S_s is the specific storage (L^{-1}), h is the potentiometric or hydraulic head (L), and t is time (T).

Similarly, reactive transport of contaminants in groundwater with uniform porosity is given by (Freeze and Cherry 1979):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial C}{\partial x_i}\right) - \frac{\partial}{\partial x_i}(v_i C) + \frac{q_s}{\theta} C_s + \sum_{k=1}^{N} R_k \qquad (2)$$

where, $i = x, y, z.$, D_{ij} = hydrodynamic dispersion coefficient (L^2T^{-1}), C = concentration of contaminant in fluid (ML^{-3}), v_i = velocity of groundwater flow at time t (LT^{-1}), θ = porosity of the porous medium, R_k = chemical reaction term, and C_s = concentration of the sources or the sinks. The movement of a conservative pollutant in a 1-D system can be expressed as:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} \qquad (3)$$

where: $\partial C/\partial t$ is the rate of change in concentration of pollutant over time.

Due to the hydrodynamic dispersion, the concentration of a contaminant will decrease over distance. Generally, a particular contaminant species will spread more in the direction of groundwater flow than in the direction normal to the groundwater flow (Cacas, *et al*., 1990), because longitudinal dispersivity is typically about 10 times higher than transverse dispersivity (Cacas, *et al.,* 1990).

The system investigated in this study can be taken as an aquifer bounded at the top by an aquitard and at the bottom by an impermeable bedrock. The aquifer–aquitard boundaries are assumed to be horizontal. The aquifer is homogeneous and horizontally isotropic (i.e. $K_x = K_y = K_z$) with constant longitudinal and transverse dispersivities (i.e. $D_{xx} = D_{yy} = D_{zz}$, and, $D_{xy} = D_{yx}$, $D_{zx} = D_{zy} = 0$).

To make predictions of some future behaviour of fluid and contaminant, the partial differential equations (Equations 1 and 2) describing ground-water flow and transport is solved mathematically using finite difference (FD) numerical methods (Konikow and Glynn, 2005).

Modelling of groundwater flow and contaminant transport

Conceptual model

The development of conceptual model was based on structural and conceptual hydrogeological model (CHM) of the study area. The CHM (Fig. 2) was developed by integrating information on the structural, geology, hydrogeology and hydraulic properties of the site. The CHM helped understand flow paths and transport mechanisms, and the development of a conceptual mathematical model for the study site.

The transport process investigated in this study takes place in a fractured permeable zone, within a rock matrix which has negligible permeability as compared to the fractured zone.

The fractured permeable zone was determined based on structural analysis and range of borehole depth values of groundwater occurrence in the study area (Darko, 2001; Yidana *et al*, 2010). Groundwater is often found to flow in only a few permeable fractures, especially in crystalline rocks (Zhao, 1998).

The approximate geometry of the problem may be represented as in Fig. 3. The origin of the coordinate system is at the upper boundary. The positive z-axis is downward. The aquifer is assumed infinite in the x- and y- directions but finite in the z-direction with a thickness of d (m). The aquifer is horizontal without curvature. A *no-flow* boundary exists at the top and bottom of the aquifer (z = d). The upper boundary is aquitard, and bottom contact is with an impermeable bedrock. The upper boundary is taken as the water table and assumed to have a small slope such that it can be assumed to be parallel to the lower boundary. The shape of the contaminant source is a parallelepiped body with $x \in [0, x_0]$, $y \in [0, y_0]$, and $z \in [z_0, z_1]$. Steady-state groundwater flow is along the x-axis. Upon applications of the simplifying assumptions, the problem reduces to a quasi-one-dimensional flow as shown in Fig. 3.

Even though the problem of study is a hetero-

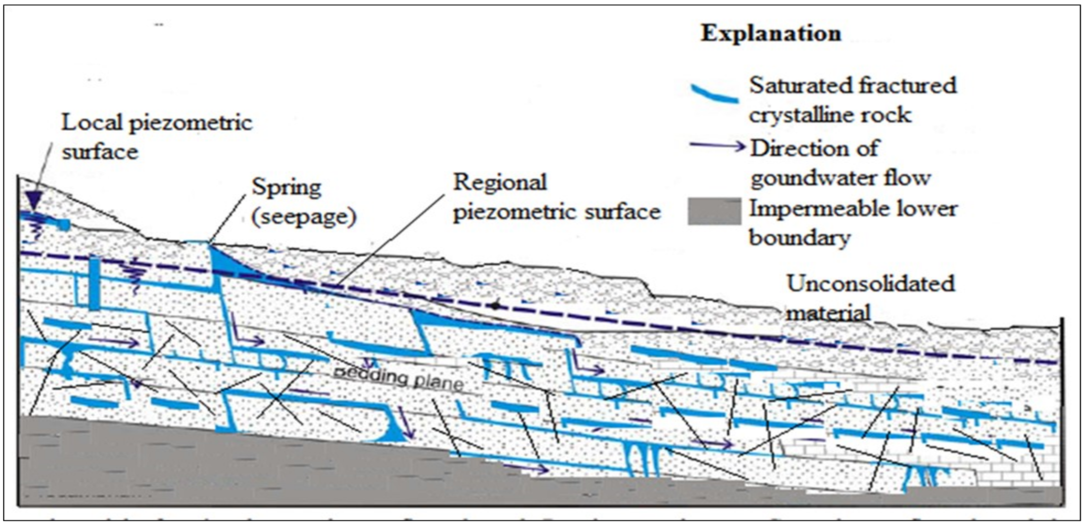

Fig. 2. Simplified conceptual hydrogeological model of the structural togo units. (Modified after, Muff and Efa, 2006: GSD and BGR, 2009)

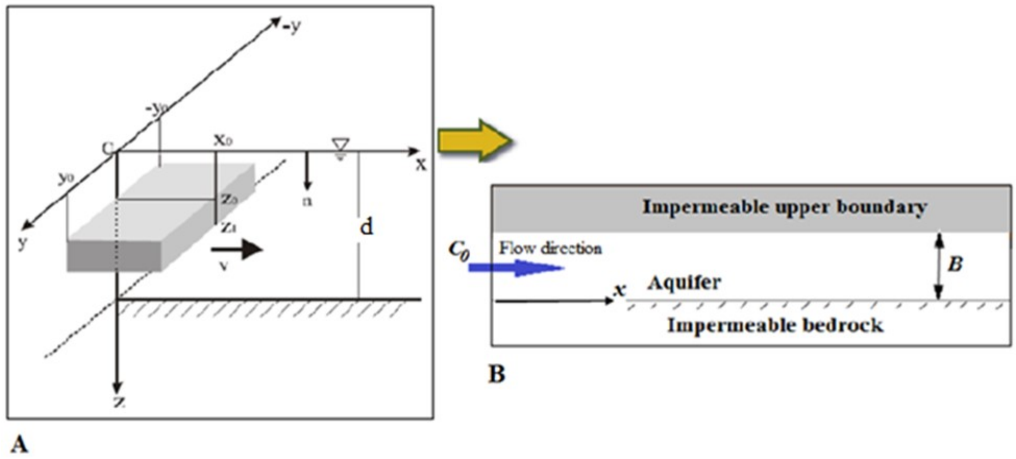

Fig. 3: Schematic diagram of the problem that is investigated, (A) 3D flow system showing direction of groundwater flow, (B) quasi-1D flow (aquifer is bounded by upper and lower no-flow contacts)

geneous system, the fracture networks are converted to three-dimensional networks of essentially one-dimensional slab consisting of open fractures that intersect each other forming the conductive network. Each fracture is assigned with a volume, size and transmissivity and simulated as deterministic or stochastic (Dershowitz and Fidelibus, 1999).

In this study, finite difference method (FDM) has been chosen to solve the advection-dispersion-equation (ADE) model of contaminant transport. This method is much simpler, though its accuracy could be compromised in higher dimensions (Gurarslan *et al*., 2013). The technique is also well suited for complex geometries, complicated flow patterns, heterogeneity, and nonlinearity (Rowe, 1988).

Simplifying assumptions

The assumptions and approximations made in this study are based on previous principal ideas of fluid models in fractured crystalline rock environment (Lomize, 1951; Romin, 1966; Nelson, 1985) and are as follows:

I. The rock matrix is idealised as large blocks of impermeable material surrounded by a network of discrete fractures along which the fluid (water) flow and contaminants travel (Bear and Berkowitz, 1987).

II. The fracture aperture (width) is much small compared with its length, allowing for a quasi-1D transport mechanism.

III. There is complete mixing across the fracture widths at all times (i.e. no change or variation in density).

IV. The domain of interest in this study is in the saturated zone of the rock mass, and is single phase fluid.

V. The contaminant is conservative (non-volatile, non-sobbing, non-degrading nor reactive).

VI. The flow is assumed laminar and the analogy of parallel planar plates is adopted to represent the fracture surfaces.

These assumptions lead to the conclusion that the main features responsible for the conduction of groundwater through the crystalline rocks in the study area are: fractures and intersections of the fractures.

Model initial and boundary conditions

The partial differential equations stated in section 2 represent only part of our model. To complete the model, there is the need to specify initial and boundary conditions. The dependent variable in the equations is the dissolved concentrations. Therefore, the initial and boundary condition equations specify the value of these concentrations at time zero and at the boundaries of the system that is being modelled. The boundaries define the hydraulic conditions at the boundary layer or system. Determination of flow boundaries was based on analysis of field data and previous information based on average water yielding capacities and depths range of boreholes drilled in the study area by various researchers (Kesse, 1985; Darko, 2001; Yidana *et al*., 2010). The model domain is depicted in Fig. 4. The flow is assumed to be only within depths of 33 and 55 m for the Study Site (within TSU). The Initial and boundary conditions of advection-dispersion transport equation are:

Initial condition:

Equations (4) and (5) are initial conditions, for the general three-dimensional models, for hydraulic head (Equation 1) and concentration of contaminant at time t = 0 (Equation 2. The equations mathematically state that the initial dissolved concentrations are constant in space at time zero.

$$h(x, y, z, t = 0) = h_i \tag{4}$$

$$C(x, y, z, t = 0) = C_i \tag{5}$$

Boundary conditions:

The main objective of this study was to predict contaminant travel in the fractured crystalline rock using conservative (nonreactive) elements. Thus, in terms of concentration, for boundary condition, the type 1 boundary condition, also known as the Dirichlet boundary condition (condition which specifies the chemical concentration at the boundary) was used. Boundary conditions can be applied over

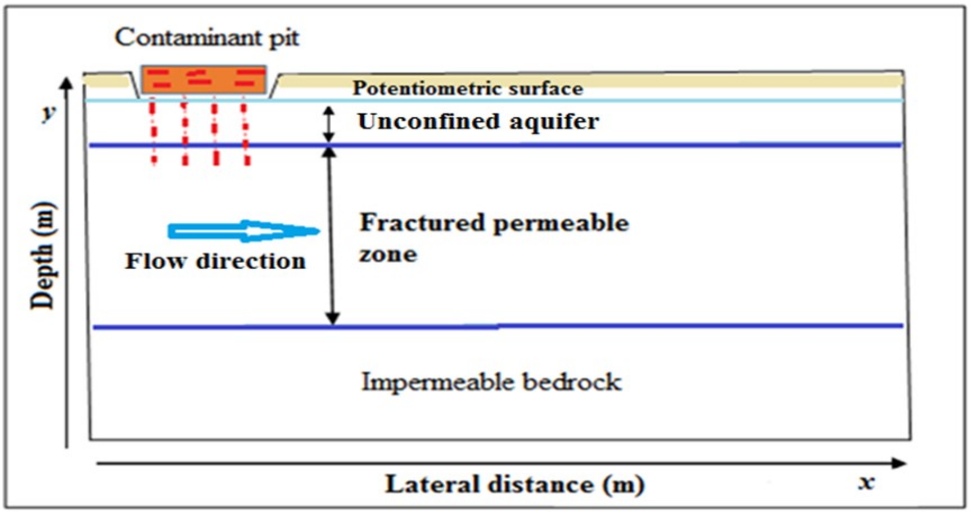

Fig. 4: Schematic diagram of the problem domain

all time ($t > 0$) or for specified time intervals ($t_1 < t < t_2$).

$$C(x, y, z, t) = C_0 \ 0 \leq x \geq x_0, 0 \leq y \geq y_0,$$
$$0 \leq y \geq y_0, t > 0 \qquad (6)$$
$$h(x, y, z, t) = h_0$$

In an attempt to determine contaminant concentration, C(x, y, and t) (dependent on position x, y and time t) in an aquifer, hydrodynamic dispersion equations are solved.

Numerical solution and predictive simulation of flow and contaminant transport

As mentioned earlier, Equation 2 and Equation 3 represent the transport of a conservative contaminant in a one- and 3-dimensional system respectively. The advection-dispersion equation may be solved analytically or numerically under different initial and boundary conditions. One of the convenient ways of obtaining numerical solutions used in simulating groundwater flow and contaminant transport through FCR is by finite-difference methods (FDM) (Anderson and Woessner, 1992).

Table 1 shows the parameter values of the model input. It gives a summary of the parameters used for the simulation of the transport of Pb (used as an example of heavy metals). Values such as hydraulic conductivity, piezometric head (or surface) and hydraulic gradient, were chosen from standard literature on the study area. These were as reported by Yidana *et al* (2010), Darko (2001) and Glover (2010). Other factors of contaminant migration for fractured rock aquifers, such as the longitudinal and transverse dispersivity and retardation factor (R) values were adopted as used by Freeze and Cherry (1979).

Fig. 4 is schematic diagram of the problem domain. The simulation was carried out for 360 days with a time step of 30 days.

Sensitivity analysis

Sensitivity analysis was carried out to investigate the effect of changes of the values for

Table 1: Input data for predictive simulation

Parameter	Value
Hydraulic conductivity (m/day)	19.4 (most permeable rock)
Hydraulic gradient	0.034 m/m
Piezometric head (above sea level)	75 m asl
Initial position of contaminant source	2.5 m (or 97.5 m asl)
Length of the reach	100.0 m
Width of the reach	100.0 m
Longitudinal dispersivity (α_L)	12.5 m
Transverse dispersivity (α_T)	1.2 m
Retardation factor	1.75
Total duration of simulation (days)	360
Time step (Δt) (days)	30
Number of divisions in length direction	20
Number of divisions in width direction	20
Initial concentration (g/m^3)	100 mg/L
Concentration at source boundary (g/m^3)	100 mg/L

hydraulic conductivity, dispersivity, partition coefficient, and retardation factor which are the main factors affected by geometric properties of fractures. This process allowed the model to be used for the possible maximum, minimum, and most probable extent of contaminant travel. The model was run for numerous iterations and the outputs were recorded at different time intervals to show the size and extent of the heavy metal and chlorite as conservative element plumes.

RESULTS AND DISCUSSION

Fig. 5(a-d) depicts the concentration contours obtained from the FDM for four different time periods. From visual inspection of the simulated contaminant plume, it can be observed that the contaminant travelled at different distance for different times. The simulated contaminant plume (Fig. 5) clearly shows the evolution of the shapes and sizes of pollution with increasing travel time. As time passes, the contaminant plume enlarges and moves along the down-gradient of the source area. The plots represent contaminant movement in two-dimension (2D). It can be observed that plume spread in the direction of groundwater flow (GF) is greater than in the direction normal to the flow because longitudinal dispersivity is typically higher than transverse dispersivity. It is also observed that

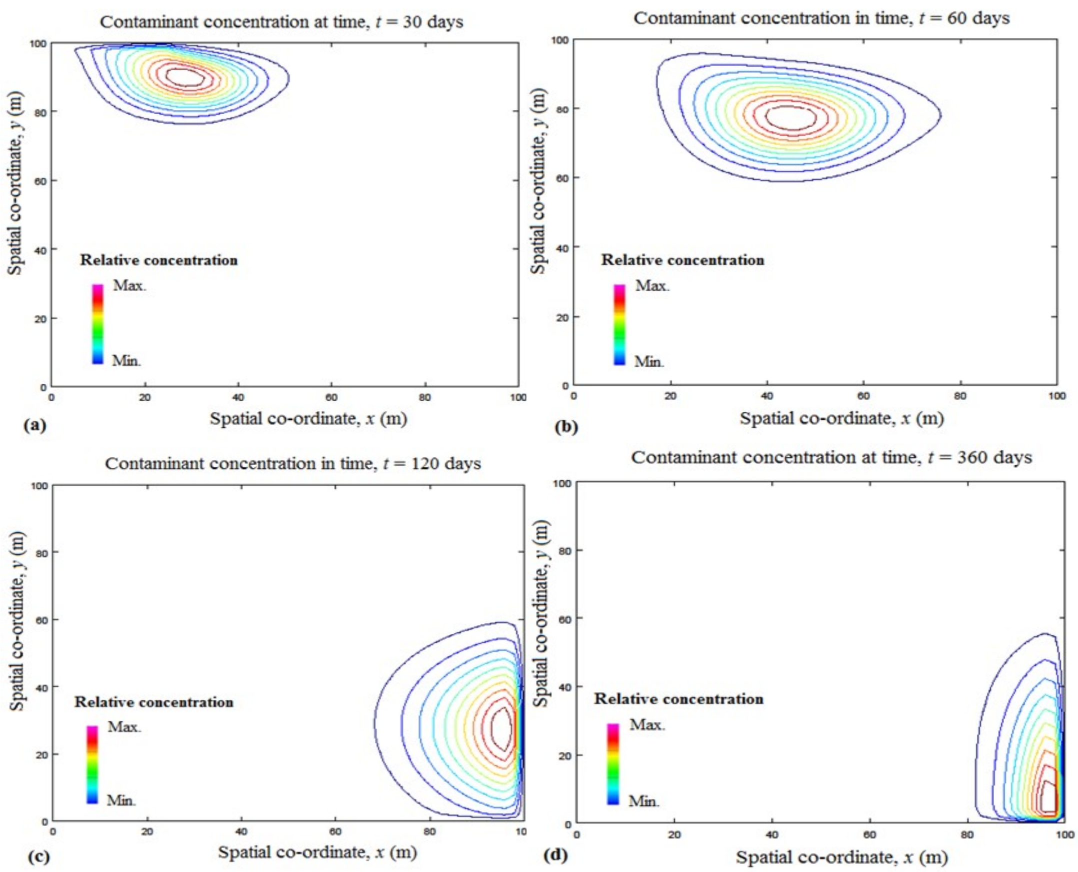

Fig. 5(a-d): Two-dimensional contour plots of contaminant plume for four different time periods: (a) time, t = 30 days; (b) time, t = 60 days; (c) time, t = 120 days, and (d) time, t = 360 days. Colours represent contaminant concentration

at the initial stage (i. e. close to the contamination source) (Fig. 5a), the size of the plume is comparatively small. Furthermore, the plots also show that contaminant migration occurs from top left (contaminant source) towards bottom right corresponding to groundwater flow direction.

Analysis of the plots indicates the contaminant can travel between 1.0 to 1.7 m/day. It is worth noting that even though this travel velocity values are low for contaminant migration for the case of a single open fracture, the values in this study represent transport in discrete fracture network (DFN), which is stochastic in nature.

The simulated contaminant transport values from this study (1.0-1.7 m/day) are comparatively high. The velocities of contaminant transport in various media have been very varied as reported from various researchers (Tang *et al,* 1981; Sudicky and Frind, 1982; Konikow and Glynn, 2010; Rao *et al*, 2013). Fallico *et al* (2012) report a velocity range from 0.06 to 1.15 m/day for porous media. In the case of crystalline rocks, Bentley and Walker (1983) determined contaminant migration in fractured dolomite as 0.3 m/day whilst Winter *et al* (1998), and Konikow and Glynn (2010) have documented ranges from about m/millennium to as high as 8 m/day. Also, comparing the transport velocity values from work done by Rao *et al* (2013), who determined contaminant travel velocity in fractured basaltic rocks in Bagalkot, India, using numerical modelling approach, and concluded that, the contaminant will be spreading in the downstream side up to a distance of about 125 m for a 5-year period, equivalent to a travel velocity of about 0.068 m/day. It can be concluded that the values determined in this study are consistent with migration contaminants in fractured crystalline rocks.

Fig. 6(a-d) illustrates the shape plots of contaminant concentration with distance in the horizontal (flow direction) for four different time intervals. From the plots, which represents the contaminants predicted movement after 360 days, it is noticed that, the contaminant is migrating from the contaminant source.

Results of the sensitivity analysis showed the model is quite stable and not changing to slight variations in most of the input parameters. Three parameters, hydraulic conductivity (K), partition coefficient and dispersivity were identified as the most dominating parameters for the contaminant transport problem.

CONCLUSION AND RECOMMENDATIONS

Mixed waste from various sources (both industrial and domestic) results in leachate generation and other processes that produce various contaminants that have the high potential of being drained into the fractured crystalline rock. This reflects a critical potential environmental hazard.

The hybrid approach appears to better describe the fluid flow and solute transport mechanism in fractured rocks at a larger field scale. FDM is presented for modelling the two-dimensional contaminant transport through the saturated fractured media. It is noted that the FDM is simple and easy to implement irrespective of size and shape of the problem domain. The results of the groundwater flow and transport simulation reveal contamination plume expansion. Contaminants could travel between 1.0 to 1.7 m/day in the horizontal direction (groundwater flow direction), indicating that, fractures are most likely responsible for contaminant migration in the typical tight sedimentary and crystalline rocks in the study area. This spreading effect of plume movement through the fractured rocks can pose critical environmental hazards.

It is highly recommended that wastes generated from various sources within urban and peri-urban areas must not be disposed of directly onto the rock formation. Engineered landfills with low permeable liner materials are advised for waste disposal site construction. New drilled and dug-out wells should be located far away from pollution sources and observation wells should be installed around waste disposal sites for periodic monitoring.

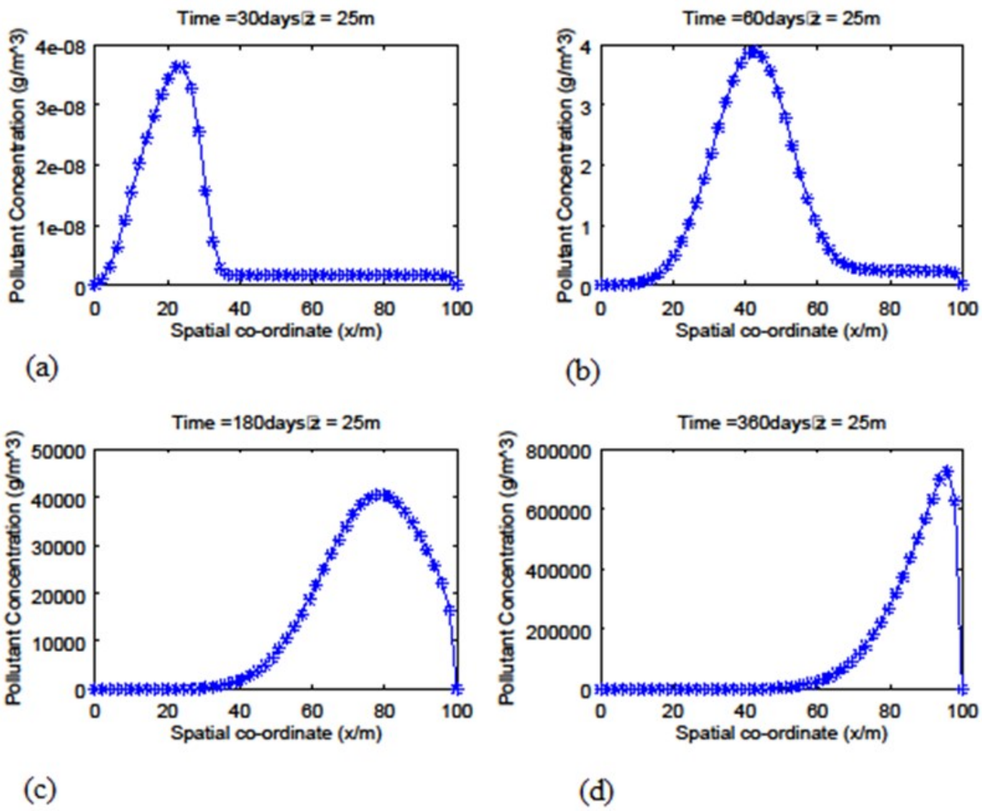

Fig. 6: Plots of Contaminant Concentration with Distance in the Horizontal (Groundwater Flow Direction) for (a): t = 30 days and z (Thickness = 25 m); (b): t = 60 days and z (thickness = 25 m); (c): t = 180 days and z (thickness = 25 m); and (d): t = 360 days and z (thickness = 25 m)

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