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Numerical modelling of contaminant transport using FEM and meshfree method

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Abstract. Groundwater contamination is seeking a lot of attention due to constant degradation of water by landfills and waste lagoons. In many cases heterogeneous soil system is encountered and hence, a finite element model is developed to solve the advection-dispersion equation for layered soil system as FEM is a robust tool for modelling problems of heterogeneity and complex geometries. Recently developed Meshfree methods have advantage of eliminating the mesh and construct approximate solutions and are observed that they perform effectively as compared to conventional FEM. In the present study, both FEM and Meshfree method are used to simulate phenomenon of contaminant transport in one dimension. The results obtained are agreeing with the values in literature and hence the model is further used for predicting the transport of contaminants. Parametric study is done by changing the dispersion coefficient, average velocity, geochemical reactions, height of leachate and height of liner for obtaining suitability.

Keywords: contaminants; drinking water; FEM and meshfree methods; landfill tech; pollutants (metals, organics, organometallics)

1. Introduction

Waste materials are stored in landfills and lagoons. Often these disposal sites are located in clay deposit or have a clay liner. Possibility of pollutant migration through these liners to nearest aquifer is of major concern. Since, the movement in such type of soils is slow and time required may range from several to hundreds of years and design of such sites require consideration of likely contamination of surrounding ground water system in both short and long term. This barrier may be underlain by a natural soil or sand which will lead to heterogeneous soil system. The key factors governing contaminant migration are advection, dispersion and chemical reaction. However, in case of clay and clay liners contaminant migration due to advective transport is smaller or negligible as compared to dispersion. Experimental studies provide a proper detailed knowledge and have been conducted to determine the parameters (Barone *et al*. 1992, Rowe and Badv 1996, Badv 2006), but actual field behaviour cannot be replicated in the laboratories and hence, the need for numerical modeling arises. These models can be used for prediction of transport for designing landfills, waste lagoons or just to observe the depleting contaminant in soil

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strata. Numerical models like finite layer method (Rowe and Booker 1984), Boundary element techniques, Finite difference method (Zhao and Töksoz 1994, Zhang *et al*. 2012), Finite element method (Gallo and Manzini 1998) have been for modeling contaminant transport equation. Finite layer technique is applicable to situations where the system is horizontally layered but aren't appropriate for situations involving complex geometry or flow pattern. Boundary element techniques are suitable for solving advection- dispersion equation and problems involving complex geometries but don't find a wide application for contaminant transport studies. Finite difference method (FDM) and Finite element method (FEM) find a broader application in the field of groundwater flow and contaminant transport. These techniques are well established and many software packages are also available. FEM provides opportunity of modeling problems with complex geometries, complicated flow patterns, heterogeneity and nonlinearity. Element free Galerkin method (EFGM) is a Meshfree method developed recently to eliminate the structure of mesh and construct approximate solutions for the equation in terms of nodes (Liu and Gu 2005). EFGM is the most successful Meshfree method and has been used for solving boundary value problems related to various field study (Belytschko *et al*. 1994, Kumar and Dodagoudar 2008, 2009). Recently Patil and Chore (2014) summarized overview of various numerical and experimental studies on contaminant transport. In the present paper, FEM and EFGM are used to model the governing differential equation for contaminant migration and a methodology is proposed for modeling one-dimensional advection-dispersion phenomenon for heterogeneous saturated media. The model is further extended for conducting parametric study to examine the effect of material constants on contaminant transport behaviour.

2. Finite element analysis

The one-dimensional form of the governing differential equation for contaminant migration through a saturated porous medium is expressed as

$$\left(1+\frac{\rho_d}{n}k_d\right)\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v_x\frac{\partial C}{\partial x} \tag{1}$$

In which, ρ_d and n are bulk density and porosity of porous medium. k_d is distribution constant. C is concentration of contaminant. D is dispersion coefficient. v_x is seepage velocity.

Initial and boundary conditions are defined as follows.

Initial condition at $t = 0$: $C = C_i$ in Ω

Boundary conditions

$$C(0,t)=C_0-\frac{1}{H_f}\int_0^t f_0(c,\tau)\,d\tau \quad \text{on } \Gamma_s \quad \text{(Dirichlet boundary condition)} \tag{2}$$

where, $f_0(c, \tau)$ is the surface flux at $z = z_0$.

H_f = Height of fluid which represents the volume of leachate

$$\frac{\partial C}{\partial x}n_s=g \quad \text{on } \Gamma_E \quad \text{(Newmann Boundary condition)} \tag{3}$$

g is zero in this case

$$\text{Ratardation factor is} \quad R = 1 + \left(\rho_d k_d / n\right) \tag{4}$$

The weighted integral form of Eq. (1) is expressed as

$$\int_0^L \left(D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - R\frac{\partial C}{\partial t} \right) dx = 0 \tag{5}$$

$$D\frac{\partial C}{\partial x} - D\int_0^L C_e^T N_x^T N_x dx C_e - v\int_0^L C_e^T N^T N_x dx C_e - R\int_0^L C_e^T N^T N dx C_e^o = 0 \tag{6}$$

$$D\int_0^L N_x^T N_x dx C_e + v\int_0^L N^T N_x dx C_e + R\int_0^L N^T N_x dx C_e^o = D\frac{\partial C}{\partial x} \tag{7}$$

$$R\int_0^L N^T N dx C_e^o \;\; + \left[D\int_0^L N_x^T N_x dx + v\int_0^L N^T N_x \right] C_e = D\frac{\partial C}{\partial x} \tag{8}$$

$$M\, C_e^{t+\Delta t} + \Delta t\left(K_1 + K_2\right) C_e^{t+\Delta t} = M\, C_e^t + D\frac{\partial C}{\partial x} \tag{9}$$

In which

$$K_1 = D\int_0^L N_x^T N_x dx\,, \quad K_2 = v\int_0^L N^T N_x dx\,, \quad M = R\int_0^L N^T N dx \tag{10}$$

$$C = N_1 C_1 + N_2 C_2 = [N]\{C_e\} \tag{11}$$

A computer program is developed in FORTRAN90 incorporating above formulation. Program is validated with comparing the results to those published in literature.

3. Element free Galerkin method

EFGM uses only set of nodes to model the boundary and generate discrete equations. It employs moving least squares (MLS) approximants formulated by Lancaster and Salkauskas (1981) to approximate the function $C(x)$with $C^h(x)$ in which $C(x)$ is the contaminant concentration at x, where x is a position coordinate. EFGM do not satisfy the Kronecker delta criterion and hence the Lagrangian multiplier technique (Dolbow and Belytschko 1998) is used to enforce the Dirichlet boundary condition.

3.1 Moving least squares approximations

According to the moving least squares proposed by Lancaster and Salkauskas (1981), the approximation $C^h(x)$ of $C(x)$is

$$C(x) \cong C^h(x) = \sum_{i=1}^{m} p_i(x) a_i(x) = P^T(x) a(x) \qquad \forall x \in \Omega \tag{12}$$

In which

$$P^T = \begin{bmatrix} 1 & x^2 \end{bmatrix} \text{ and } a^T(x) = [a_0(x), a_1(x), a_2(x) \ldots a_m(x)] \tag{13}$$

where $p(x)$ is a monomial basis function and $a(x)$ is a vector of undetermined coefficients, whose values can vary according to the position of x in Ω and m is the order of the basis.

To determine $a(x)$, we minimize with respect to $a(x)$ the weighted, discrete L_2 norm given by

$$J = \sum_{I=1}^{n} w(x - x_I)\left[C_L^h(x_I, x) - C_I\right]^2 = \sum_{I=1}^{n} w(x - x_I)\left[P^T(x_I) a(x) - C_I\right]^2 \tag{14}$$

where n is the number of nodes in neighbourhood of x for which weight function $w(x\text{-}x_I)$ is non-zero and C_I refers to nodal parameter of C at $x = x_I$

The minimum of J in Eq. (14) with respect to $a(x)$ leads to the following set of linear equations

$$A(x) a(x) = B(x) u \tag{15}$$

or

$$a(x) = A^{-1}(x) B(x) u \tag{16}$$

where

$$\begin{aligned} A &= \sum_{I=1}^{n} w(x - x_I) P(x_I) P^T(x) \\ &= w(x - x_1)\begin{bmatrix} 1 & x_1 \\ x_1 & x_1^2 \end{bmatrix} + w(x - x_2)\begin{bmatrix} 1 & x_2 \\ x_2 & x_2^2 \end{bmatrix} + w(x - x_1)\begin{bmatrix} 1 & x_3 \\ x_3 & x_3^2 \end{bmatrix} + \ldots\ldots\ldots w(x - x_1)\begin{bmatrix} 1 & x_n \\ x_n & x_n^2 \end{bmatrix} \end{aligned} \tag{17}$$

$$B(x) = w(x - x_1)\begin{bmatrix} 1 \\ x_1 \end{bmatrix} w(x - x_2)\begin{bmatrix} 1 \\ x_2 \end{bmatrix} w(x - x_3)\begin{bmatrix} 1 \\ x_3 \end{bmatrix} \ldots w(x - x_n)\begin{bmatrix} 1 \\ x_n \end{bmatrix} \tag{18}$$

$$C^T = \{C_1, C_2, \ldots C_n\} \tag{19}$$

By substituting Eq. (16) in Eq. (12), the MLS approximants can be defined as

$$C^h(x) = \sum_{I=1}^{n} \phi_I(x) C_I = \phi(x) C \tag{20}$$

where, $\Phi_I(x)$ is shape function defined as

$$\phi_I(x) = \sum_{j=0}^{m} p_j(x)(A^{-1}(x) B(x))_{JI} = P^T A^{-1} B_I \tag{21}$$

where m is the order of polynomial $p(x)$.

Derivative of shape function are obtained by

$$\begin{aligned}\phi_{I,x} &= (P^T A^{-1} B_I),x \\ &= P_{,x}^T A^{-1} B_I + P^T (A^{-1})_{,x} B_I + P^T A^{-1} B_{I,x}\end{aligned} \tag{22}$$

where

$$B_{I,x}(x) = \frac{dw}{dx}(x - x_I)\, p(x_I) \tag{23}$$

and

$$A^{-1}{}_{,x} \quad \text{is computed by} \quad A^{-1}{}_{,x} = -A^{-1} A_{,x} A^{-1} \tag{24}$$

where

$$\begin{aligned}A_{,x} &= \sum_{I=1}^{n} w(x - x_I) P(x_I) P^T(x) \\ &= \frac{dw}{dx}(x - x_1)\begin{bmatrix} 1 & x_1 \\ x_1 & x_1^2 \end{bmatrix} + \frac{dw}{dx}(x - x_2)\begin{bmatrix} 1 & x_2 \\ x_2 & x_2^2 \end{bmatrix} \\ &+ \frac{dw}{dx}(x - x_3)\begin{bmatrix} 1 & x_3 \\ x_3 & x_3^2 \end{bmatrix} + \dots\dots\dots \frac{dw}{dx}(x - x_n)\begin{bmatrix} 1 & x_n \\ x_n & x_n^2 \end{bmatrix}\end{aligned} \tag{25}$$

EFGM shape functions do not satisfy the Kronecker delta criterion $\Phi_I(xJ) \neq \delta_{IJ}$. Therefore they are not interpolants, and the name approximants is used. For imposing essential boundary conditions Lagrangian multipliers are used (Belytschko *et al*. 1994).

3.2 Weight function description

An important ingredient in EFG method is the weight function used Eq. (17). The weight function is non-zero over a small neighbourhood of x_I, called support domains. The weight function should be smooth and continuous. The choice of weight function affects the approximation results. Present study considers quartic spline function given by

$$w(x - x_I) = \begin{Bmatrix} 1 - 6r_i^2 + 8r_i^3 - 3r_i^4 & \mathrm{r_i} \leq 1 \\ 0 & \mathrm{r_i} > 1 \end{Bmatrix} \tag{26}$$

where $d_i = ||x\text{-}x_I||$ and $r = d_I/d_{mI}$, where d_{mI} is the size of domain of influence of I^{th} node. The size of the domain of influence at node, d_{mI} is computed by

$$d_{mI} = d_{\max} C_I \tag{27}$$

where, $= d_{\max}$ is a scaling parameter which is typically 2.0-4.0 for static analysis. The distance c_I is determined by searching for enough neighbour nodes for A to be regular.

The derivatives for weight function are as follows

$$\frac{dw}{dx}(x - x_I) = \begin{Bmatrix} (-12r_i + 24r_i^2 - 12r_i^3)\ sign(x - x_I) & r_i \leq 1 \\ 0 & r_i > 1 \end{Bmatrix} \tag{28}$$

The discretisation of the governing equation mentioned in Eq. (1) is done similar to the finite element method

Only following changes are observed

$$\begin{bmatrix} K & G \\ G^T & 0 \end{bmatrix} \begin{Bmatrix} c \\ \lambda \end{Bmatrix} = \begin{bmatrix} f \\ q \end{bmatrix} \tag{29}$$

In which

$$\begin{aligned} & K = K_{IJ}^{*}\ \Delta t + M_{IJ} \\ & K_{IJ}^{*} = \int_0^L \left[\phi_{I,x}^T D \phi_{J,x} + \phi_I^T v \phi_{J,x} \right] dx \quad and \quad M_{IJ} = \int_0^L \left[\phi_I R \phi_J \right] dx \\ & q_K = C_{0K} \quad and \quad f = M\{C\} + \Delta t\ \{Q\} \\ & G_{IK} = -\Phi_K \quad on\ \left| \Gamma_{sI} \right. \quad ; \quad Q_I = -\Phi_I D_g \quad on \left| \Gamma_E \right. \end{aligned} \tag{30}$$

4. Validation

Validation of the results obtained is done with the experimental results of Rowe and Booker

Table 1 Material Properties from Rowe and Booker (1984)

Parameter	
Dispersion constant D (m^2/year)	0.01
Average velocity for 1st layer (m/year)	0.00166
Advection velocity for 2nd layer (m/year)	25
Length of clay liner and natural soil (m)	3.0 and 1.0
Dispersivity (m)	0.1
Time (years)	115
Time step (years)	0.05
Porosity n_1 and n_2	0.4 and 0.35
Height of leachate H_f(m)	1.0
Bulk density of soil and distribution constant ρK	0.0

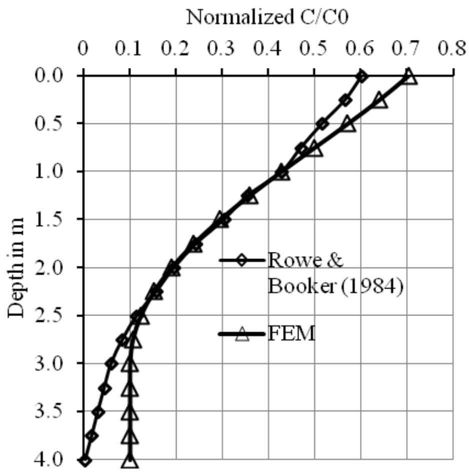

Fig. 1 Validation of FEM results with Rowe and Booker (1984)

Table 2 Material Properties from Sharma *et al*. (2014)

Parameter	
Dispersion constant *D* for 1st (cm^2/hour)	40
Dispersion constant *D* for 2nd (cm^2/hour)	5
Average velocity for 1stand 2nd layer (cm/hr)	10
Length of clay liner and natural soil (cm)	60
Time (hour)	1
Dispersion constant *D* for 1st (cm^2/hour)	40
Dispersion constant *D* for 2nd (cm^2/hour)	5

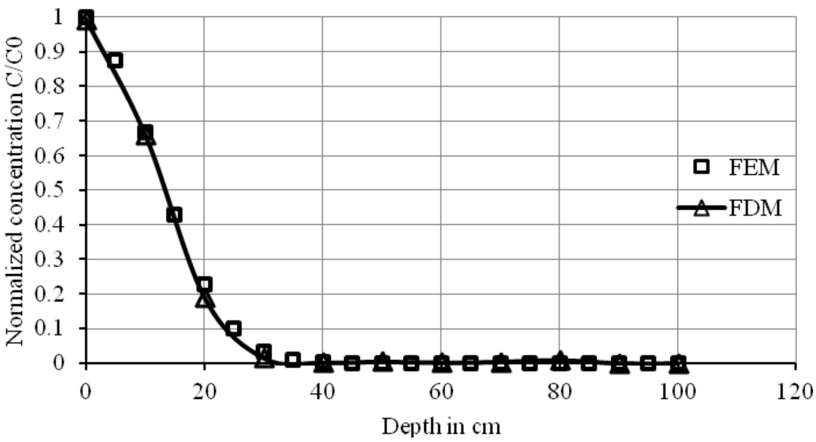

Fig. 2 Validation of FEM results with Sharma *et al*. (2013)

(1984). The material properties are reported in Table 1. Variation of normalized concentration along depth is depicted in Fig. 1 along with the experimental results. It is observed that the results obtained from FEM model are in close agreement with the experimental results. Results confirm that the finite element program is in agreement with the values in literature and can be used for further research.

Further, FEM program was validated with the values mentioned in Sharma *et al*. (2014). Sharma *et al*. (2014) have used FDM for solving the differential equation for heterogeneous media. The material properties are reported in Table 2. It is observed that the results obtained from FEM model are in close agreement with FDM results.

5. Comparison of FEM and EFGM

EFGM formulation was further used to develop a program in FORTRAN 90. The material properties used are reported in Table 3. Total of 11 nodes were used. The results obtained agreed well with the FEM results.

Table 3 Material properties

Parameter	
Dispersion constant D for 1st (m^2/hour)	0.1
Dispersion constant D for 2nd (m^2/hour)	0.01
Average velocity v for 1st (m/hr)	0.5
Average velocity v for 2nd (m/hr)	0.1
Length of clay liner and natural soil (m)	1

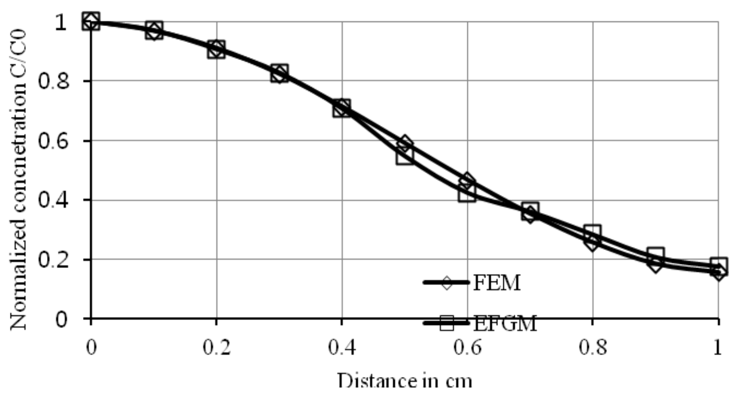

Fig. 3 Validation of EFGM results with FEM results in heterogeneous media

Fig. 4 depicts the normalized concentration profiles with distance for values of the shape parameter (d_{max}). It can be seen that the values of d_{max} equal to 2.1 show stable results and the same shall be used for further analysis.

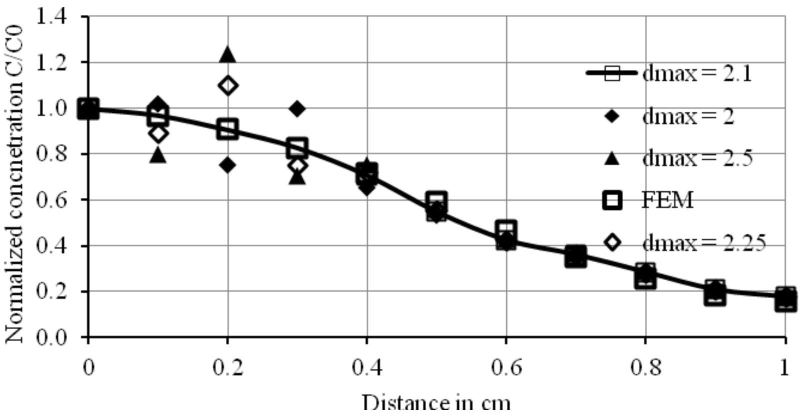

Fig. 4 Normalized concentration values for different values of d_{max}

6. Parametric study

After assuring the accuracy of the program, study is extended to examine the effect of change in dispersion coefficient, average velocity and change in depth.

6.1 Effect of change of dispersion

Dispersion is the apparent mixing and spreading of the contaminant within the flow system which is given by

$$D_L = a_L.V + D^*$$

where D_L = Dispersion coefficient (L^2T^{-1}), a_L = Dispersivity (L), V = average velocity (LT^{-1})

D^* = Molecular Diffusion (L^2T^{-1})

Dispersion is due to mechanical mixing and molecular diffusion. The mixing component, often called mechanical dispersion arises from velocity variations in porous media and dispersivity. Dispersivity varies from 0.1 to 100 m. An approximate value for dispersivity is 0.1 times the scale of test (Gelhar *et al*. 1992). Molecular diffusion is process where ionic or molecular constituents move in the direction of their concentration gradients. The values of D^* range from 5×10^{-6} to 20×10^{-6} cm^2/s with smallest value associated with ion having greatest charge. The diffusion coefficients of Mg^+, Ca^+, K^+, Na^+, Cl^- are given as 0.0222 m^2/year, 0.025008 m^2/year, 0.061811 m^2/year, 0.041943 m^2/year, 0.012 m^2/year (Shackelford and Daniel 1991, Rowe and Sawicki 1992, Schwartz and Zhang 2012). In Fig. 5, variation in normalized concentration along depth for different values of Dispersion is presented while keeping all the other values same as in Table 1. An advective layer lies underneath the clay liner and it is observed that if the sorption or geochemical reaction i.e., ρK is zero and then reduction in concentration of pollutants doesn't occur for pollutants having higher diffusion coefficients.

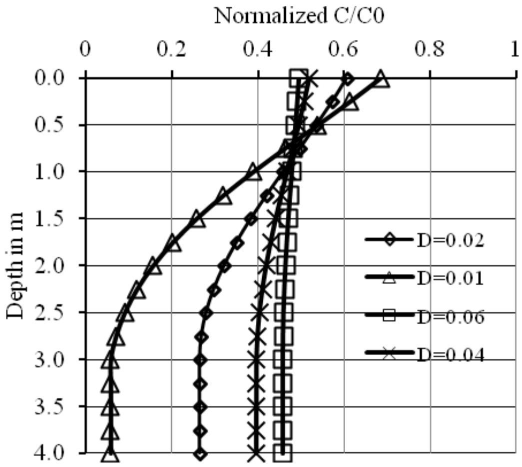

Fig. 5 Effect of change of dispersion coefficient

6.2 Effect of change of average velocity

Advection is the movement of the contaminant due to flow of water within the flow system. It is the main process conveying dissolved mass from one point to another. Velocity change implies that the material property of the top layer in the landfill is changed and the velocity below the top layer will remain same as the landfill is constructed on the natural soil. Hence values of velocity of

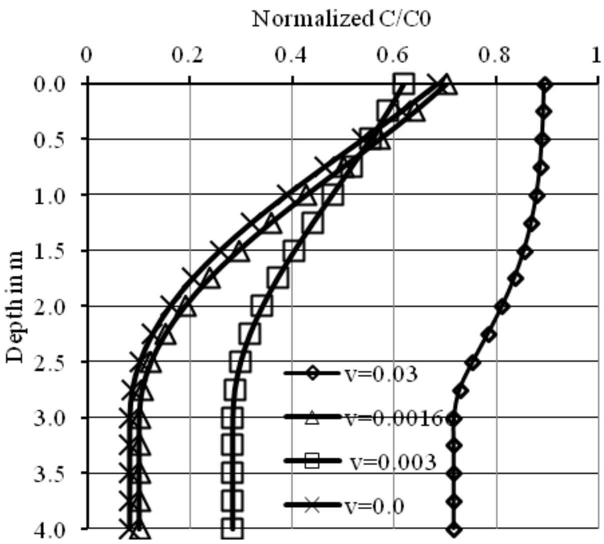

Fig. 6 Effect of change of advective of velocity of top layer

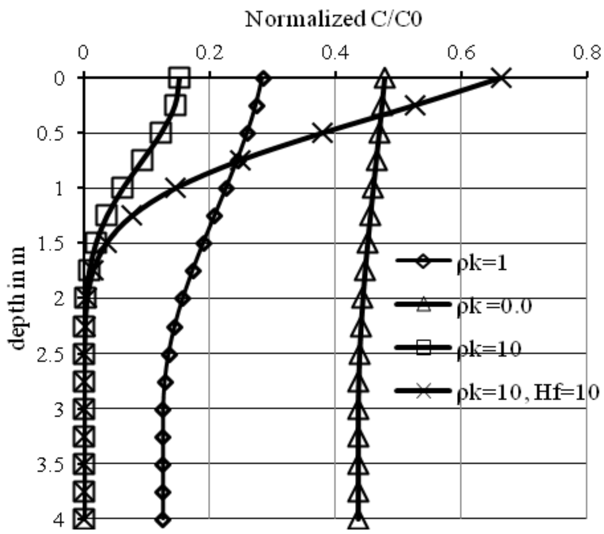

Fig. 7 Parametric changes on normalized concentration

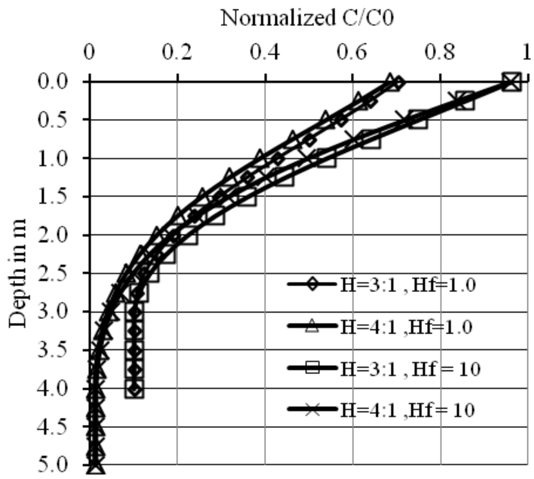

Fig. 8 Effect of change of depth of top layer

only top layer will change. This is done to check the effect on transport of contaminant this parametric study is done. Values of only velocity are changed and rest values are the same as in Table 1.

Fig. 6 shows the effect of change in velocity. It is observed that 0.03 m/year velocity is relatively large and dominated by advection and such situation arises when there is a failure of leachate collection system. Usually, a velocity less than 0.03 m/year will be encountered. As it is observed that negligible or zero velocity is most favourable for condition for reducing pollutant concentration.

Fig. 7 shows that for reducing concentration having a high diffusion coefficient, geochemical reaction ρK should be greater than zero and if height of leachate is less, the concentration with respect to depth depletes but even if the height of leachate is more than 10m or even infinite, with geochemical reaction, concentration can reduce with respect to depth.

6.3 Effect of change of depth of the liner

Effect of change in depth of liner by maintaining all other values (as given in Table 1) is observed to check the flow of contaminant transport along the depth. The effect of clay liner with 3m height and 4m height is obtained and shown in Fig. 5. It is observed that with increase in liner height, concentration with respect to depth is reduced. Height of leachate H_f also plays an important role. If it is less than 10 m then contaminant transport depletes with respect to height and vice versa. But in some cases H_f has to be equal to infinity, but in such cases also increasing the height of clay liner improves the results.

7. Conclusions

From the above analysis, FEM and EFGM can be used for modelling contaminant transport in heterogeneous media and can be used for predicting the future of contaminant migration in landfill liners. Further, EFGM results are validated using results obtained by FEM and are in good agreement. Parametric study for observing depletion of concentration by changing the dispersion coefficient, average velocity, geochemical reactions, height of leachate and height of liner is performed. It is observed from it that, geochemical reactions and height of leachate play an important role in depleting the concentrations. Two and three dimensional contaminant transport modelling are desirable in order to have proper understanding of contaminant migration.

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